REPORT DOCUMENTATION PAGE

Form Approved OMB NO. 0704-0188

1. REPORT DATE (DD-MM-YYYY): 27-05-2016

2. REPORT TYPE: Final Report

3. DATES COVERED (From - To): 1-Feb-2015 - 31-Jan-2016

4. TITLE AND SUBTITLE: Final Report: X-ray Diffraction System for Advanced Materials Analysis in Research and Education

5a. CONTRACT NUMBER: W911NF-15-1-0025

5b. GRANT NUMBER:

5c. PROGRAM ELEMENT NUMBER: 106012

5d. PROJECT NUMBER:

5e. TASK NUMBER:

5f. WORK UNIT NUMBER:

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8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS (ES)
U.S. Army Research Office
P.O. Box 12211
Research Triangle Park, NC 27709-2211

10. SPONSOR/MONITOR'S ACRONYM(S): ARO

11. SPONSOR/MONITOR'S REPORT NUMBER(S): 66343-EL-REP.1

12. DISTRIBUTION AVAILABILITY STATEMENT
Approved for Public Release; Distribution Unlimited

13. SUPPLEMENTARY NOTES
The views, opinions and/or findings contained in this report are those of the author(s) and should not contrued as an official Department of the Army position, policy or decision, unless so designated by other documentation.

14. ABSTRACT
Funds were received and expended to acquire the Rigaku SmartLab high-resolution x-ray diffraction (XRD) system with HyPix-3000 array detector. The SmartLab is suitable for user-friendly measurement reconfiguration to analyze thin films, powders, and nanomaterials. The acquisition supports current materials research at Texas State University, a Hispanic serving institution, and will support future research initiatives based on a 5-year warranty and broad base of university funding to projects. The system is emerging as a major resource in the existing Analysis Research Service Center (RSC), a fee-based user facility which ensures broad access to instrumentation.

15. SUBJECT TERMS
x-ray diffraction system acquisition

16. SECURITY CLASSIFICATION OF: a. REPORT	b. ABSTRACT	c. THIS PAGE	17. LIMITATION OF ABSTRACT	15. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
UU	UU	UU	UU		Mark Holtz
					19b. TELEPHONE NUMBER 512-245-4720

Standard Form 298 (Rev 8/98)
Prescribed by ANSI Std. Z39.18

Report Title

Final Report: X-ray Diffraction System for Advanced Materials Analysis in Research and Education

ABSTRACT

Funds were received and expended to acquire the Rigaku SmartLab high-resolution x-ray diffraction (XRD) system with HyPix-3000 array detector. The SmartLab is suitable for user-friendly measurement reconfiguration to analyze thin films, powders, and nanomaterials. The acquisition supports current materials research at Texas State University, a Hispanic serving institution, and will support future research initiatives based on a 5-year warranty and broad base of university funding to projects. The system is emerging as a major resource in the existing Analysis Research Service Center (RSC), a fee-based user facility which ensures broad access to instrumentation.
The XRD complements extensive materials growth and device fabrication RSCs for conducting research supported by federal, state, and industry funding. This support currently includes four Department of Defense awards. The new XRD system replaced an antiquated, single-investigator system acquired in 1994 for thin-film analysis. The state-of-the-art SmartLab system provides new capabilities and reduces measurement time to allow expanded user-ship for both research and education.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Received Paper

TOTAL:

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

Received Paper

TOTAL:

Number of Papers published in non peer-reviewed journals:

(c) Presentations

Number of Presentations: 0.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received Paper

TOTAL:

Number of Manuscripts:

Books

Received Book

TOTAL:

Received Book Chapter

TOTAL:

Patents Submitted

Patents Awarded

Awards

Graduate Students

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Faculty Supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:...... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:...... 0.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):...... 0.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:...... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields:...... 0.00

Names of Personnel receiving masters degrees

NAME

Total Number:

Names of personnel receiving PHDs

NAME

Total Number:

Names of other research staff

NAME	PERCENT_SUPPORTED

FTE Equivalent:
Total Number:

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

See Attachment.

Technology Transfer

N/A

Final Report for W911NF1510025
Proposal 66343-EL-REP

"X-ray Diffraction System for Advanced Materials Analysis in Research and Education"

Texas State University

Principal Investigator

Mark Holtz

Support Personnel

Gary Beall, Chemistry & MSE

Ravi Droopad and Qingkai Yu, Eng. & MSE,

Tom Myers, Edwin Piner, and Nikoleta Theodoropoulou, Physics & MSE

Technical Support Personnel

Eric Schires and Casey Smith

Prepared May 21, 2016

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Overview

Funds were received and expended to acquire the Rigaku SmartLab high-resolution x-ray diffraction (XRD) system with HyPix-3000 array detector. The SmartLab is suitable for user-friendly measurement reconfiguration to analyze thin films, powders, and nanomaterials. The acquisition supports current materials research at Texas State University, a Hispanic serving institution, and will support future research initiatives based on a 5-year warranty and broad base of university funding to projects. The system is emerging as a major resource in the existing Analysis Research Service Center (RSC), a fee-based user facility which ensures broad access to instrumentation.

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Selection and Purchasing Process

The selection process began with an overview of available vendors and preparation of a document articulating our system needs. The document is included as **Appendix 1**.

This document was distributed to PANalytical Inc., Rigaku Corp., Jordan Valley Semiconductor LTD, and Bruker Corp. with an estimate of budget. Of these four, Jordan Valley opted out of the selection process.

To pre-screen each of the remaining vendors, we carried out a combination of on-site and video conferences with them at the university. Following these initial discussions, and assurance by each vendor that they could provide a capable system that was affordable to us, we produced an array of testing samples to send to each vendor, all receiving the same set, so that they could carry out measurements to be returned to each investigator for evaluation.

The set of samples to evaluate was:

- GaN HEMT structures
- CdTe double heterostructures
- Organic Semiconductors
- STO/BTO, STO/Si
- Copper nano-composite
- Additional as warranted for follow-up

All three vendors were capable of providing acceptable data on all samples. Data provided by the successful Rigaku system are included as **Appendix 2**.

Purchase followed university guidelines, established by the State of Texas, which required a quote or bid from each vendor. Based on qualifications and cost, we decided to obtain the Rigaku SmartLab with an anticipated delivery in December, 2015. The final quotation, with system specifications, is included as **Appendix 3**.

Following issue of the purchase order to Rigaku, Dr. Casey Smith and Mr. Eric Schires visited Rigaku to go through their general training. Dr. Smith is technical director of our Nanofabrication user facility.[1] Mr. Schires is technical director of the Analysis Research Service Center.[2] These personnel are central figures in our oversight and training efforts in materials science and engineering, and extensively cross-train to ensure facility stability and operation.

In addition to the complete XRD system, full analysis software is standard as part of the purchase to support all measurement capabilities. We also negotiated 10 licenses so that data analysis could be carried out off-line from the XRD. Further shrewd negotiation allowed us to add the Anton Paar DHS 1100 Domed Hot Stage to the purchase for investigations from ambient temperature to 1100 °C. The final purchase left $300 balance which we supplemented to purchase a large-screen television and PC table. The large-screen television is directly connected to the SmartLab PC and has proven to be very useful for training and outreach activities.

Installation, Qualification, and Training

Delivery took place the first week of January, due to shipping time and university closure for the winter holiday. Rigaku personnel were on site that same day and for approximately one week to install and qualify the system. Installation included modifying the power drop in the laboratory, handled by university electricians, and required resolving minor plumbing connection compatibilities. At that point, final payment was issued for the system.

Rigaku training was scheduled for February to allow university personnel time to work with the system and develop questions related to specific needs and applications. Dr. Aya Takase conducted the on-site training. Directly involved in the training were Dr. Casey Smith and Mr. Eric Schires, along with Mr. Pete Walker who functions as the student super-user. Mr. Walker handles routine training and day-to-day assistance to users.

[1] http://www.msec.txstate.edu/Research/Facilities-and-Instrumentation/Nanofabrication.html
[2] http://www.msec.txstate.edu/Research/Facilities-and-Instrumentation/Analysis.html

Photographs of the Rigaku SmartLab system funded by this award. Site preparation, move in, and placement followed by photographs of the system post installation. The equipment is located in the Roy F. Mitte building where the majority of Analysis Research Service Center equipment is housed.

Administration

The Rigaku SmartLab is administratively operated by the Analysis Research Service Center. The PI of this project is chairs the Steering Committee of the Analysis Research Service Center. This user facility provides training and access university wide and to outside users. This structure ensures broad usership of equipment and qualifies it for repairs under the Provost’s Shared

Equipment Fund. The ARSC has approximately 140 current users. The fee structure currently allows for three levels:

- Type A: Internal user based on grant or contract funding directly to the university.
- Type B: External user funding work done on campus with exchange of intellectual property and publication of outcomes.
- Type C: External user with no exchange of intellectual property.

Note that any federal SBIR/STTR contract with the university automatically qualifies as Type A.

The fee structure includes four instrumentation levels. The SmartLab is at Level IV, the highest, with internal user rate of $35/h. The Analysis Research Service Center functions on a cost-replacement basis and is not permitted to generate or retain a surplus. To ensure that the Center operates on cost-replacement, the rates are reviewed twice each year and adjusted accordingly. Adjustments do not affect the hourly, rather the monthly project cap is adjusted. The cap for Type A users is currently $498/mo.

Impact on Research

The Rigaku SmartLab has already had an important impact on materials research. To date, 38 users have been trained to use the equipment corresponding to 14 projects. We expect this to grow. Here we include reports from a few projects.

Selective Growth of Diamond for Thermal Management

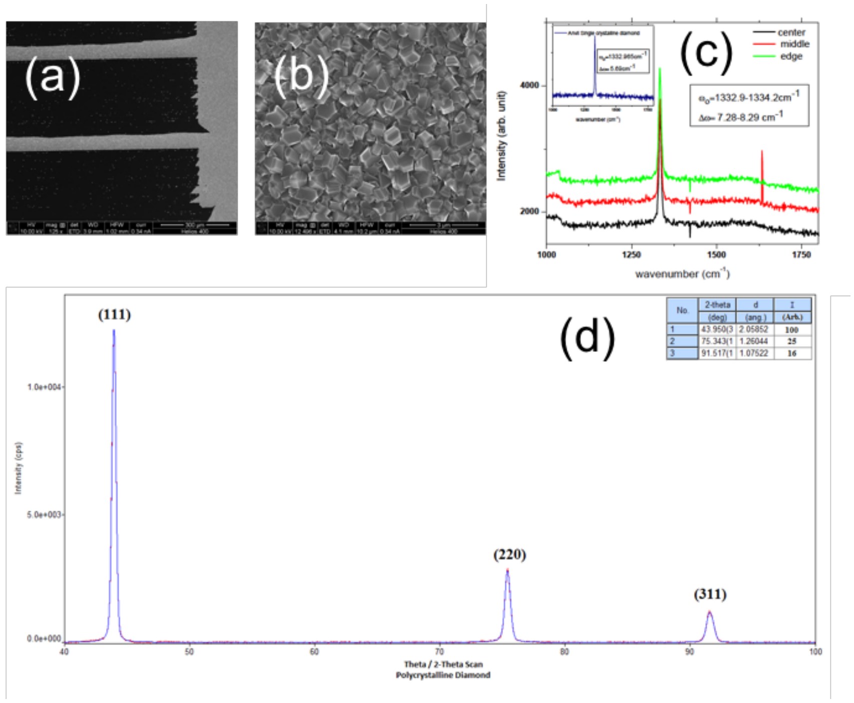
We are engaged in systematic investigations of diamond-on-GaN for heat spreader implementation in III-nitride semiconductor transistor structures. Studies involve material growth, characterization, design and measurement of electrothermal test structures, and simulations to understand the effect of materials and interfaces on thermal management.

The overarching goal is to reduce the impact of self-heating that degrades performance and accelerates device failure. The principle route to mitigating this problem is implementation of diamond as a heat spreader. However, full integration of III-nitride epitaxy with diamond deposition requires in-depth study of the process steps and their impact on material aspects of the structure, particularly the interfaces formed between the layers.

An innovative path to thermal management is described through selective diamond growth on GaN, to be implemented in close proximity to the two-dimensional electron gas (2DEG) channel in an AlGaN/GaN heterostructure. Selective growth is promising for controlling diamond polycrystallinity and concomitant effects on thermal conductivity (κ) and thermal boundary resistance (TBR), as well as mitigating in-plane stress.

We have initiated selective growth of diamond on test silicon wafers. The approach (unpublished) leverages prior work in using photoresists to disperse and pattern diamond nano-seeds. Standard spin coating was used for seeding the wafers. Seeding uniformity was analyzed using scanning electron microscopy (SEM). The seeded wafer was loaded in the Crystallume CVD diamond chamber at Texas State University. This hot filament CVD reactor utilizes 9 tungsten wires of 0.01 inch diameter for current and voltage of 100 A and 63 V, respectively. Step one was to establish uniform seeding and growth, which was accomplished using the cleanroom of our Nanofabrication Facility. The figure entitled Diamond SEM & Raman shows

some early results. The approach developed to seed and grow diamond resulted in selective growth as demonstrated by the SEM image (a). Although the lateral size is close to 100 μm, due to the photomask used in this demonstration, the surrounding fields are relatively free from diamond growth. SEM (b) shows the morphology of the diamonds to be typical of CVD growth. The Raman spectra in (c) show narrow diamond O(Γ) scatter at 1332 cm^{-1}, indicating high quality, and low non-diamond-carbon intensity (broad feature near 1600 cm^{-1}). The latter is indicative of a low volume fraction of disordered carbon in the polycrystalline matrix, which is critical for good thermal properties.



Diamond SEM & Raman. (a) SEM image demonstrates early selective growth success. (b) SEM image showing polycrystalline morphology. (c) Micro-Raman spectra showing good diamond quality and low non-diamond-carbon volume fraction. (d) θ-2θ pattern of CVD polycrystalline diamond.

θ-2θ scan measurements were performed on CVD grown polycrystalline diamond on Silicon (111) over a range from 40° to 100°, as shown in panel (d). The three most intense peaks are shown with a consistent lattice spacing of 0.3565 nm. This data was measured in parallel beam mode with a 5° parallel slit analyzer using a Cu X-ray source and Kβ filter.

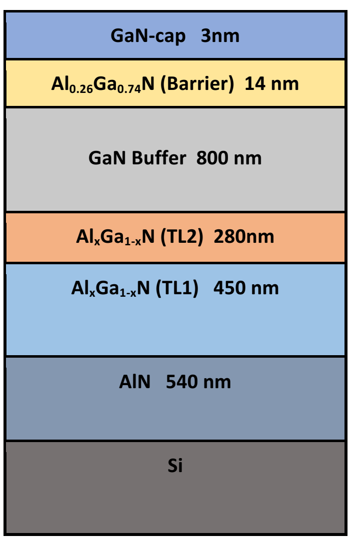
MOCVD Growth of AlGaN/GaN

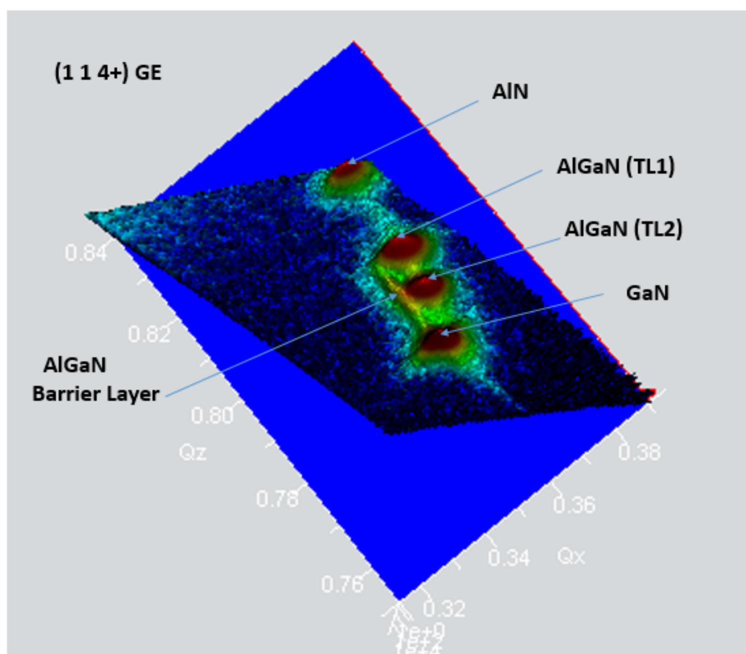
X-ray crystallography is a state of the art non-destructive technique to determine crystal structures, defects, interface roughness, thickness and composition of the semiconducting material. Using our 4-inch capable Metal Organic Chemical Vapor Depostion (MOCVD) system, we in our group, typically grow III-N based AlGaN/GaN high electron mobility transistor (HEMTs) heterostructure. See Figure MOCVD(a). We are extensively using our Rigaku SmartLab system to characterize various structural and morphological parameters. HRXRD with two-bounce Ge(002) monochromator is being used to get the rocking-curve

measurement for GaN buffer layer for symmetric (0 0 2) plane and Triple axis coupled (2θ-ω) scan to find the peaks for different (AlGaN) transition layers (TL) and AlN layers. Analyzing these data using Globalfit Software and other calculation we can determine the crystalline quality and c-lattice constant for various layers in the HEMT structure. Moreover Al% composition of fully relaxed layer like (TL1 and TL2) can also be calculated from (0 0 2) reflection.

Since we have a pseudomorphically strained barrier layer, which has almost the same Al% as the TL2, symmetric reflection of (002) can't reveal distinctive barrier layer peak. To find the barrier layer's compositions and crystalline quality we are using (reciprocal space map) RSM measurement for different asymmetric mainly (1 1 4) and (2 0 5) to find barrier peak hence the lattice constant both a, and c. Figure MOCVD(b) is a 3D topography representation of RSM measurement for GaN (1 1 4) with Grazing Exit (GE) geometry. Here, the barrier layer peak is very evident. Using strain corrected Vegard's law Al% of barrier layer is determined. Strain and relaxation of different layer are also being calculated using simulation software as well as calculation.

The thickness and interface roughness of the barrier layer is very crucial forming desired 2DEG hence overall device performance. Acquiring the XRR data and simulate it in the Globalfit software we can determined the thickness of the GaN cap (~3nm) and barrier layer (~ 14 nm) and the interface roughness as well. To fit the data we use the determined Al% from the RSM measurement to get exact thickness data. Taking advantage of the Rigaku *X-Y* stage we can also map the whole wafer for thickness and Al% compositions.

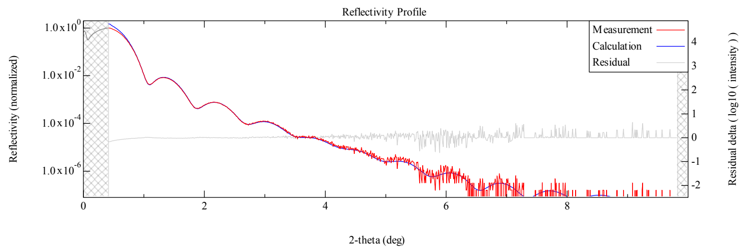




MOCVD. (a) Schematic of AlGaN/GaN HEMTs (not drawn to the scale) heterostructure. (b) 3D topography representation of RSM for asymmetric (1 1 4) plane with GE geometry.

MBE Growth of Functional Oxides

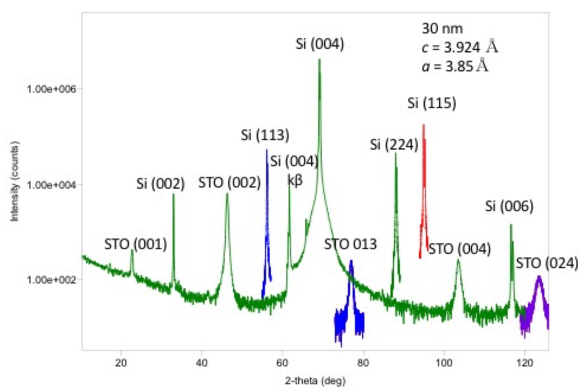
The newly installed XRD system has had significant impact on the NSF-CAREER project (PI Theodoropoulou). Under this project she is investigating growth of oxide materials by molecular beam epitaxy (MBE) where one of the challenges is correctly determining the stoichiometry of the oxides, such as $SrTiO_3$, $BiFeO_3$, by adjusting the temperature of each of the cells (sources)



Results

ID	Material	Thickness (nm)	Density (g/cm3)	Roughness (nm)
2	STO	9.91688	4.95816	0.409515
1	STO	0.981787	2.88052	0.699222
Sub.	Si	0.0[--]	2.33[--]	0[--]

Oxide XRR. X-ray reflectivity measurements and fitting results for $SrTiO_3$ layer.



Automated XRD. Automated XRD scan over many different symmetric and asymmetric peaks.

which is required for successful growth. This is especially important to the project because we are measuring magnetotransport properties due to carriers originating from oxygen vacancies. Charge carriers can also originate from non-stoichiometry. For example, a few percent excess Ti over Sr results in additional electrons that dominate the transport properties.

The SmartLab automated alignment procedures allow for very fast, routine measurements of the thickness using x-ray reflectrometry (XRR), as shown in the figure **Oxide XRR**. These measurements have allowed improvements in oxide growth process using up-to-date growth rates and hence enable better source calibration. Additionally, the XRR modeling software program has helped reveal a less dense interfacial layer on some of the samples. This layer is

expected under certain conditions as it depends on the exact growth parameters. The results are also be seen with TEM cross-sections, which are time intensive and costly. The capability of the XRD system has improved both our growth success ration rate and the level of parameter control.

We have also used scripting and automatic alignments to determine the *a*, *b*, and *c* lattice constants. These measurements were fairly difficult with the outdated Bede D1 since the chi adjustments were imprecise and unrepeatable thus rendering any asymmetric alignments and scans nearly impossible. The figure **Automated XRD** shows the result of an automated scan over many different symmetric and asymmetric peaks that were done using the scripting feature and the diffraction space simulation to find each peak. These are very repeatable measurements thanks to the automated alignment and the precision of the chi stepper motor which we did not previously have. The accurate determination of the crystal parameters is very important in correlating electric and magnetic transport properties with strain and oxygen deficiency.

High-Resolution XRD of CdTe-CdMgTe Double Heterostructures

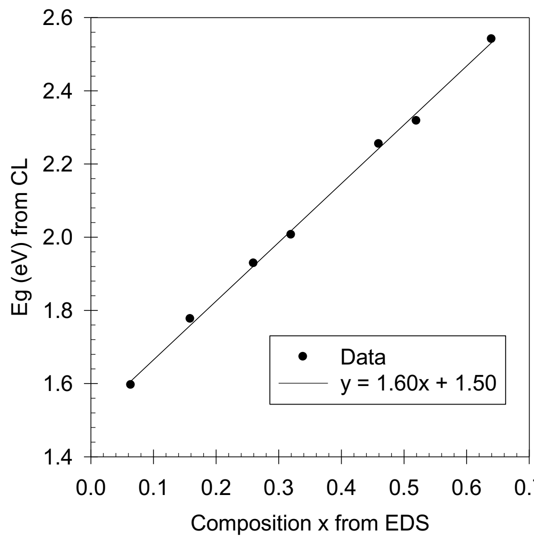
Multilayer heterostructures are often used as device or materials diagnostic structures. The determination of the composition and thickness of various component layers is typically carried out utilizing high-resolution X-ray diffraction (HR-XRD) using the "known" lattice parameters and elastic constants elastic constants of the constituents.

This has routinely been performed recently for CMgTe/CdTe double heterojunctions used to probe fundamental properties of CdTe and interfaces between CdTe and other materials with the goal of improving the knowledge base for photovoltaics for solar cells, and SWIR detectors.

We also decided to establish a second method for determining CdMgTe alloy content as that helps lower the number of free parameters in the HRXRD analysis. In multiple thick $Cd_{1-x}Mg_xTe$ films, x was measured by energy dispersive X-ray spectroscopy (EDS), and E_g was measured by cathodoluminescence (CL). In double heterostructures, the thin CdMgTe barriers had their E_g measured by variable angle SE in the range 250-800 nm, at incident angles of 65°, 70°, and 75°.

- Magnesium composition

The Mg composition x in the barrier layers is shown as a function of the peak luminescence from CL in figure **Energy gap vs Composition**. The resulting linear regression yields a relationship that is, within three significant figures, identical to one of the previously reported composition versus band gap relationships, which was generated by a comparison of ellipsometry values for E_g to X-ray photoemission spectroscopy (XPS) values for x.



Energy gap vs Composition. The cathodoluminescence peak from a double heterostructure barrier is compared to the Mg composition from energy dispersive spectroscopy.

We used this relationship to derive x for CdMgTe barriers within a double heterostructure based on E_g. The band gap E_g was in turn measured by SE. The band gaps of II-VI alloys have been determined by employing SE along with various parametric models. The particular model used here specifies a three layer structure – a 10nm cap layer of CdTe, a 30 nm top barrier of CdMgTe, and a CdTe substrate which is treated as semi-infinite, since the absorption coefficient of CdTe prevents light from penetrating through the 0.5-5 micron absorber layer to the bottom CdMgTe barrier and returning. The complex index of refraction of CdTe at each wavelength is fixed at values taken from the literature. This approach allowed us to quantify the alloy composition of the top CdMgTe barrier. Interestingly, using this alloy value resulted in HRXRD-determined thicknesses different from what we believed based on growth parameters.

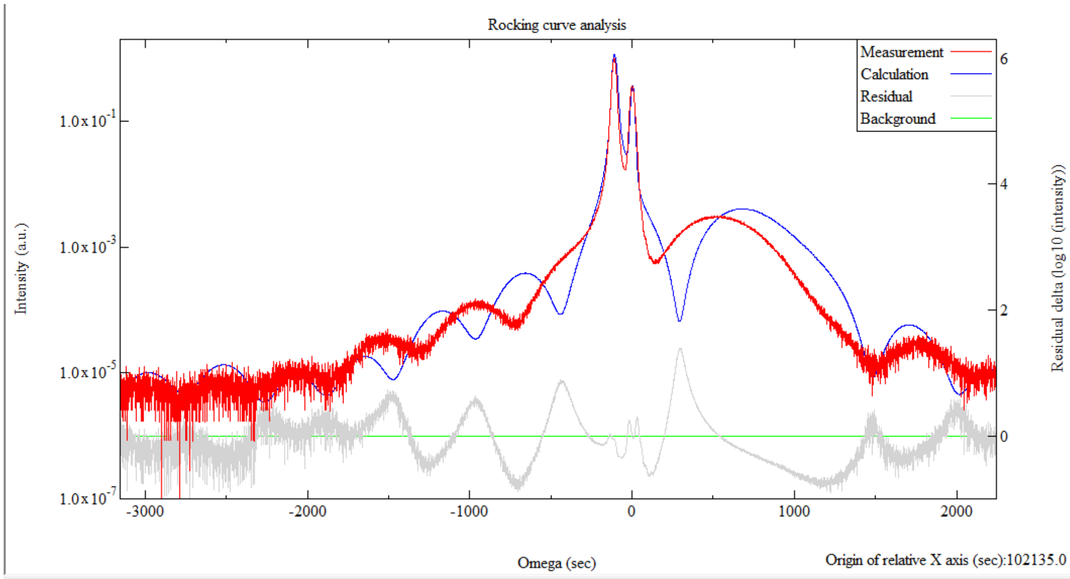
During the course of work performed on a subcontract : "High Quality CdTe and Alloy Growth by Molecular Beam Epitaxy (MBE)" for prime contract "Approaching the S-Q Limit with Epitaxial CdTe" with the *Alliance for Sustainable Energy, LLC Management and Operating Contractor for the National Renewable Energy Laboratory (NREL)*, quite a few samples had the various layer thicknesses directly measured by transmission electron microscopy and the barrier composition measured using atom probe tomography in partnership with Dr. Brian Gorman's group at the Colorado School of Mines. Interestingly, the composition of the barriers agreed well with the determination made by SE. One result of the measured values is shown in figure **CdTe/CdMgTe DH**.

Top HJ Thickness	27.5
Bottom HJ Thickness	27.5
CdTe Middle Layer Thickness	955
CdTe epi layer thickness	1032
Mg content, x=	0.376

CdTe/CdMgTe DH. Parameters measured for a CdTe/CdMgTe DH grown on a CdTe buffer layer on InSb by MBE. The thicknesses (in nm) were measured from TEM images such at that shown on the right. The composition was determine using atom probe tomography, shown in the middle.

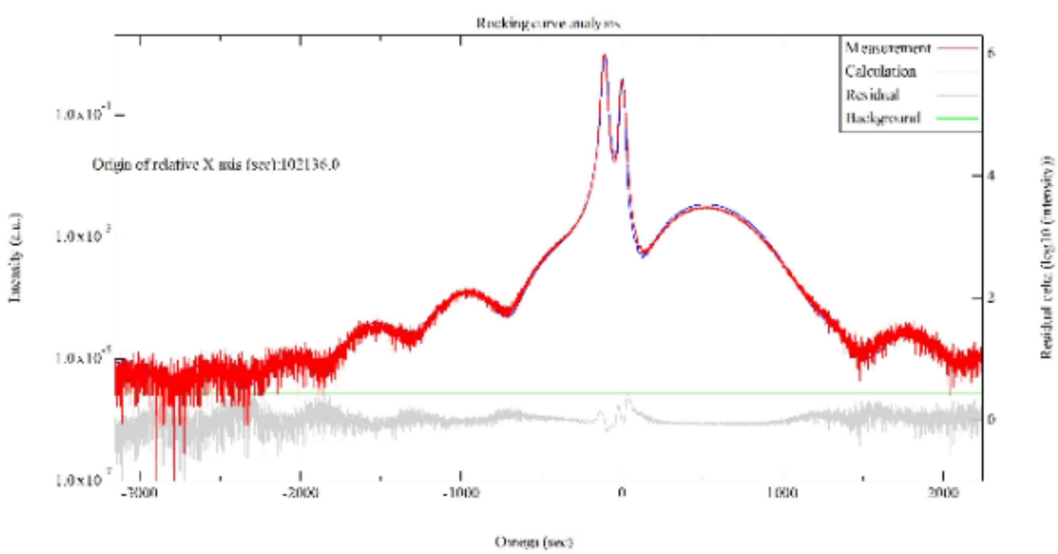
Unfortunately, when we used these measured parameters and tried to use the appropriate HRXRD models, we found rather poor correlation as indicated in figure **HRXRD DH Model**. The other inputs were the elastic constants and lattice parameters for CdTe and InSb, which are well established, and the published lattice parameter value for MgTe with a linear interpolation between CdTe and MgTe elastic constants. This strongly suggests that prior studies using only these latter inputs and modeling thicknesses and composition In this system likely leads to erroneous results.

By modifying slightly the CdMgTe input parameters, a good fit of the data can be obtained as indicated in figure **HRXRD DH Improved Model**. However, we have only looked at two samples of approximately the same composition and layer thicknesses, and so are not ready to suggest "improved" values for CdMgTe. However, we have fifteen high structural quality DHs that have undergone SE, TEM and APT measurement with varying layer thicknesses and CdMgTe compositions. We plan this summer to use this somewhat unique sample set to establish better values for the MgTe lattice parameter endpoint, and CdMgTe elastic constants.



	Top CdMgTe Layer	Bottom CdMgTe layer	Absorber	buffer	ATP	SE
Z 323	27.50nm	27.50nm	955 nm	1032 nm	X=0.376	X=0.37

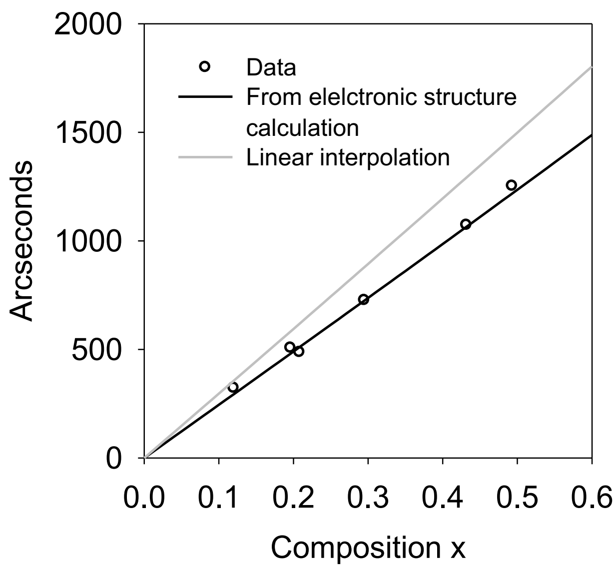
HRXRD DH Model. Comparison of using measured thicknesses and compositions to model the HRXRD data, as opposed to fitting as free parameters, poor correlation was observed. Note the consistency of the SE and ATP determination of x for CdMgTe.



HRXRD DH Improved Model. Improved fit occurring with a small change in MgTe lattice parameter or elastic constants (or both).

Further complications are suggested by the information shown in **Deviations from Vegard**. The lattice mismatch between the CdMgTe and the CdTe results in in-plane strain, which leads to a change in the growth axis lattice spacing, as determined by Poisson's ratio. This growth axis spacing can be measured by HRXRD. By taking the variation with x in elastic constants from our recent electronic structure calculation that suggests linear interpolation is not valid, and noting the specific formula for Poisson's ratio applying to growth in the 211 direction, we obtain the model results shown in figure **Deviations from Vegard**. The barriers of our DHs grown on (211) CdTe substrates match the predictions well. If the elastic constants are instead calculated by linear interpolation between the standard values of CdTe and MgTe, the match is poor, indicating that the elastic constants of CdMgTe do not obey a simple Vegard's Law relationship.

We plan to utilize the highly characterized samples at our disposal to improve the understanding of the CdMgTe system with HRXRD measurements.



Deviations from Vegard. Difference in arc-seconds between the HRXRD CdMgTe peak and the substrate peak for heterostructures grown on (211) CdTe.

Impact on Education

Formal courses utilize the XRD system to broaden its impact on education. These courses have are important because they prepare students for industry and, as they move to more research-intensive work, the original work they will conduct as MS and PhD students.

In Spring Semester 2016 students in courses were trained to use the SmartLab, as shown in Table 1. Course syllabi are included as **Appendix 4**. The Thin Films Laboratory course is project oriented with significant creative input by the student teams. Professional development is emphasized including a formal poster session at the end of the semester. For most students, this is their first experience presenting in poster format, and the "battle hardening" gained during this activity prepares them well for professional conferences. The Materials Characterization course

is required for our PhD program in Materials Science, Engineering, and Commercialization. More details are below. In both courses, students are engaged in rigorous training of principles and measurements, plus ample hands-on training. One outcome of this course is the identification of student super-users who will serve as trainers on instrumentation in the Analysis Research Service Center. This duty is part of their Doctoral Instructional Assistantship and provides for them additional expertise in various characterization methods.

Table 1 Courses incorporating hands-on training of Rigaku SmartLab.

Course Number & Title	Instructor	Number of Students
PHYS5324 Thin Films Laboratory & MSEC7310: Nanoscale systems and devices	Dr. Zakhidov	16
MSEC7311 Materials Characterization	Dr. Theodoropoulou	12

The system was used in MSEC 7311 course with graduate students from several different departments in the College of Science and Engineering: Biology, Materials Science Engineering and Commercialization Ph.D. program, Electrical Engineering, Manufacturing Engineering and Engineering Technology. XRD was one of the five instruments students were trained to use and implement for a Lab assignment and their Final project. The students worked in rotating teams of 2-3 people completing five different Lab assignments.

Here is an excerpt from the MSEC 7311 XRD laboratory assignment:

You are given a Si wafer with a thin film of a certain metal deposited on top and a plain Si wafer Your objective is 4-fold:

a. Determine the type of film that is deposited on Si, i.e. what is the element?
b. What is the thickness of the film?
c. What is the crystal orientation of the Si substrate?
d. What is the off-cut of the Si substrate?

Your report should include:

1. XRD spectra with all the peaks clearly identified and labeled.
2. If you have fittings to your data, identify all the fitting parameters and their significance and their importance on the fit (how sensitive is your fit on the parameters?)
3. Explain clearly and succinctly your experimental procedures, do not include "recipes" but rather explain which parameters you are optimizing and how (theta, chi…)

In your report answer the following questions:

- Is there an Oxide or interfacial layer
- Is there noise in your measurements? Why? What is the background on your spectra?
- Are there any artifacts? What are they and how can you reduce them?

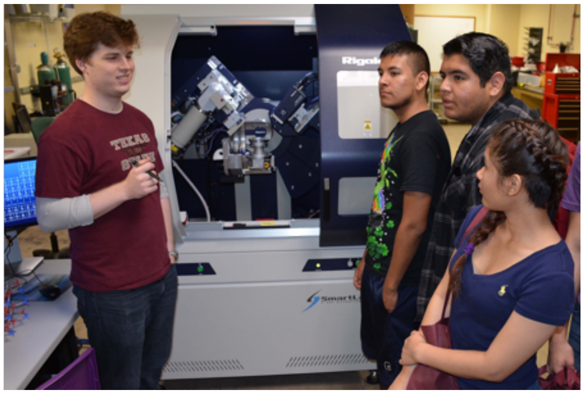
For the final project, each teams of students were given an unknown powder sample and were asked to use all the available instruments to characterize it and identify it. They were also asked to assess its commercial potential as a sunscreen and agree on the product with the most potential for this applications. The samples were mixed nanoparticle powders of ZnO, TiO_2 and CeO_2, 15-30 nm diameter nanoparticles.

In Fall Semester PHYS 5322 "Semiconductor Device Microfabrication" and MSEC7360 "Nanomaterials Processing" will be offered. Students will be trained in XRD using the SmartLab.

Outreach

The Analysis Research Service Center routinely hosts groups for outreach visits. In Spring Semester 2016 regional schools with active chapters of the Society for the Advancement of Chicanos/Hispanics and Native Americans in the Sciences (https://sacnas.org/). We anticipate many more such activities. In Summer 2016 two workshops are planned in the PI's department and the Analysis Research Service Center will be heavily involved in tutorials on materials research and tours of facilities including demonstrations of the SmartLab.

- Research Experience for Science Teachers: Nanotechnology in Everyday Life is funded through the NSF CAREER Grant (http://www.txstate.edu/physics/NT-REST.html), Dr. Theodoropoulou PI. The Research Experience for Science Teachers workshop is ideally suited for High School and Middle school teachers of any STEM discipline. Participants are immersed in a university research environment for one week over the summer, the theme of the annual workshop is "Science in Everyday Life" focusing on Nanotechnology.
- Meson Physics Camp: STEM Engagement for Middle Grades, Leadership Development for High School & Texas State Students (Halliburton Foundation Grant), Dr. E. Close, PI. This is a summer physics camp for middle school students. Faculty work with undergraduate students to create and test engaging hands-on curriculum, recruit and enroll 80-100 middle school students from San Marcos CISD, recruit and mentor high school physics students as junior camp counselors, and coordinating logistics with San Marcos CISD and Mathworks Junior Math Camps.



Photos of one SACNAS group during visit to Texas State University and the Analysis Research Service Center XRD facility.

Appendix 1
System Specifications sent to Prospective Vendors

X-ray diffraction system for materials analysis
Texas State University

1. Fully enclosed and interlocked diffractometer, electronics rack, system controller and software. Suitable for university user-based facility.
2. Theta-Theta goniometer capable of diverse measurements for materials analysis: semiconductors, nanoparticles, liquids.
3. X-ray tube: Cu anode with power rating at least 1.8 kW. Designed for use with X-ray mirrors, hybrid and Johansson monochromators. Windows for line and point focus.
4. Non-spinning sample stages:
    a. For 1 mm capillaries
    b. Tooling necessary for filling and using capillaries
    c. Solids and powder holders for 2D SAXS
    d. Powder holder inserts (3)
    e. 2D SAXS kit (Masks for 2D SAXS)
    f. Attachment for SAXS and WAXS under low vacuum conditions. Two anti-scatter slits, capsule for different sample holder types, semi-transparent beam-stop, vacuum interface. Wide angle range SAXS/WAXS to at least 79 degrees in 2Theta.
5. Sample stages with tilt capability
    a. Quarter-circle cradle with programmable chi, phi, and z motions. Ranges at least: chi -3 to 93 deg, phi 2 x 360 deg, z 64 mm. Samples to at least 2 kg in mass, 140 mm diameter, and 64 mm height.
    b. At least 140 mm sample table
    c. Clamping system for sample holder
    d. Manual xy stage for 3-axis cradle. Sample mass to at least 1.5 kg, l x w x h at least 95 mm x 95 mm x 51 mm. Positioning range at least 54 mm both axes. Sample diameter at least 80 mm.
    e. Accessories for easy sample height adjustment.
6. Sample stages for low/mid temperature.
7. Incident beam optics for line focus
    a. Soller slit 0.04 radians exchangeable with Soller slits 0.01, 0.02, or 0.08 radians
    b. Bragg-Brentano divergent-beam optics with energy resolution to 450 eV (requires replacing incident beam Ni beta filter). Fixed divergence slit holder and antiscatter devices for FDS, Soller slits holder, attenuator.
    c. Set of beam masks to reduce width from X-ray mirror and hybrid monochromators.
    d. Small angle scatter slit: incident fixed slit for beam optics such as mirror, hybrid/focusing mirror to limit size of incident beam.
8. Incident beam optics for line focus base on monochromators and hybrids
    a. 2 bounce hybrid monochromator: X-ray mirror and two-crystal Ge (220) two-bounce monochromator for Cu K-alpha-1. Discrimination

    to K-alpha-2 at least 0.1%. FWHM of Si(111) reflection < 0.007 degrees.
   b. Soller slit holder for 8a hybrid monochromator.
   c. Beam mask set (4 ranging from 20 to 2 mm).
9. Diffraction beam optics (collimators)
   a. High-resolution rocking curve optics
      i. Receiving slits of 1, 1.5 and 0.4 mm (1 and 1/4 degrees) and a beam mask of 1 mm. 90 degree slit holder rotation providing a horizontal or vertical slit.
   b. 3 bounce Ge monochromator.
   c. Soller slit 0.04 radians, large aperture for diffracted beam anti-scatter device for X'Celerator detector. Exchangeable with Soller slit 0.02 radians.
10. Detector
    a. Array detector with high dynamic range for use as point, line, or area detector
       i. At least 256 x 256 pixel array
       ii. ~ 55 μ pixel size,
       iii. 97% count rate linearity to 50,000 cps per pixel or 12,800,000 cps per strip.
       iv. Scanning and static 2D functionality and 3D computed tomography functionality
    b. Static 2theta range of 3.3 degrees.
    c. Large diffracted beam Ni Beta filter for array detector and for parallel plate collimators. For Cu radiation.
    d. Fixed Antiscatter slit assembly for the PIXcel detector. Includes slits (13.4, 11.2, 7.5 and 6mm) and alignment slit.
    e. Soller slit 0.04 radians, large aperture for diffracted beam anti-scatter
11. Programmable beam attenuator
12. Brand name computer (Dell or equivalent) for controlling system. Network compatible.
13. Full analysis software package to support data collection and interpretation. Support simulation and fitting software. Competitive renewal/update policies.
14. Water-to-water heat exchanger. Connection lines, flow meter, strainer compatible with standard plumbing fittings.
15. Air filtration kit from compressed air lines to unit.
16. On-site training.
17. Installation.
18. Quote should include full instrument coverage for 5 years. This can be a combination of initial warrantee and extended service contract.
19. Shipping included.

Appendix 2
Data Provided by Rigaku from several of our Samples

SmartLab
X-RAY DIFFRACTOMETER

XRD analysis report

Prepared for: Texas State University

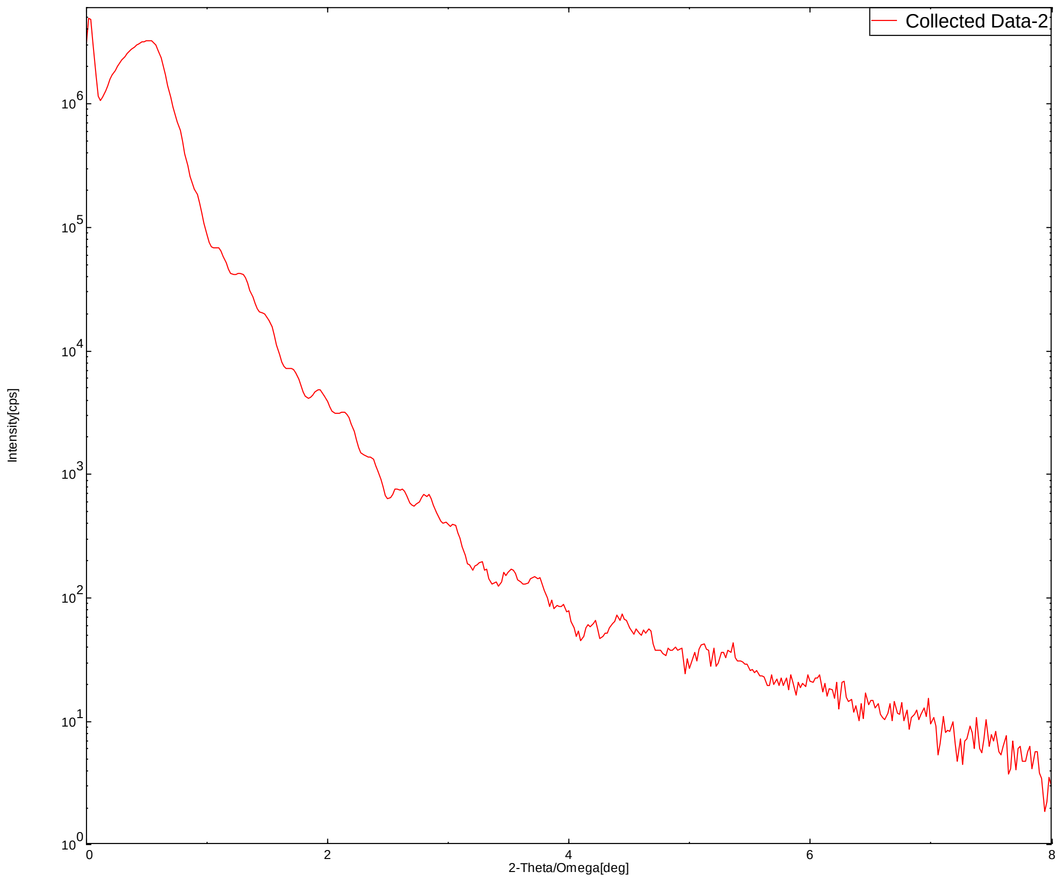
Prepared by: Aya Takase (aya.takase@rigaku.com)

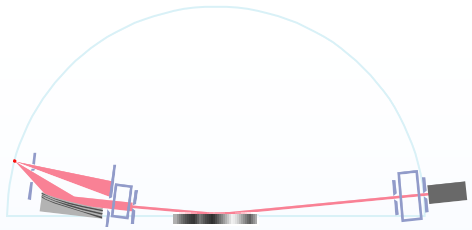
April 10, 2015

Rigaku
Leading With Innovation

2359 / reflectivity raw data

Parallel beam for XRR – HyPix3000 0D



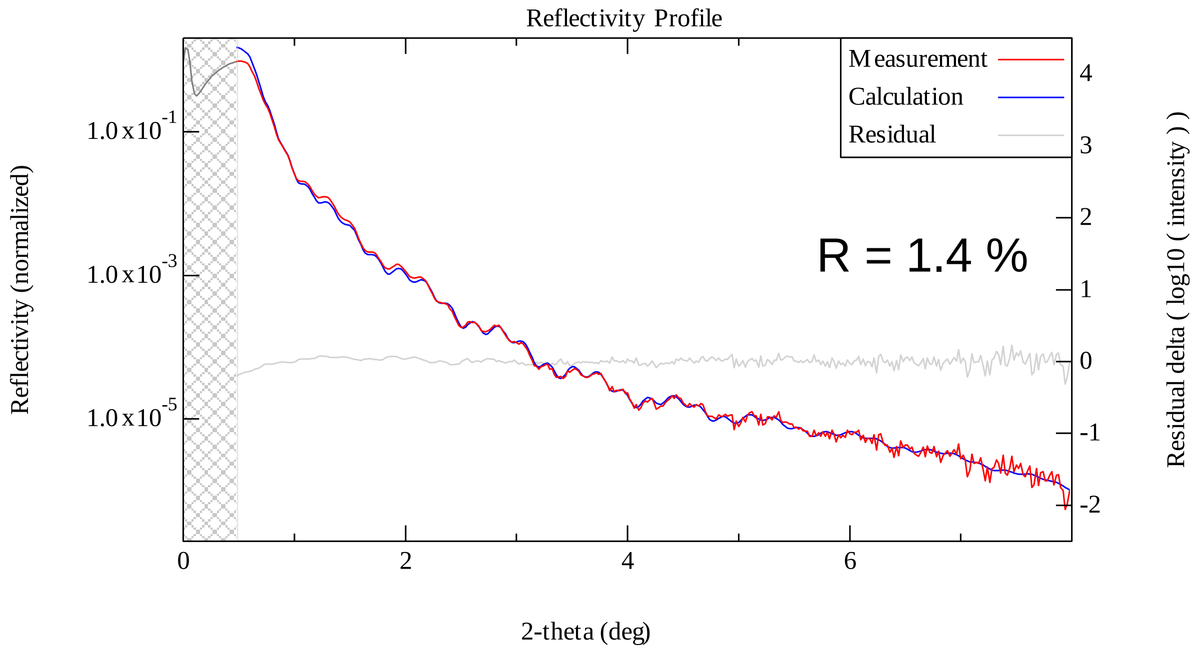


SmartLab / Standard
Parallel beam

Att.:	Standard
Detector:	HyPix3000 0D
XG:	40 kV – 44 mA
SI:	0.1 x 5 mm
Soller S.:	5 º
RS1:	0.25 mm
RS2:	0.35 mm
Axis:	θ / 2θ scan
Range:	0.0 – 8.0 º
Step:	0.02 º
Speed:	0.4 º / min

2359 / reflectivity analysis

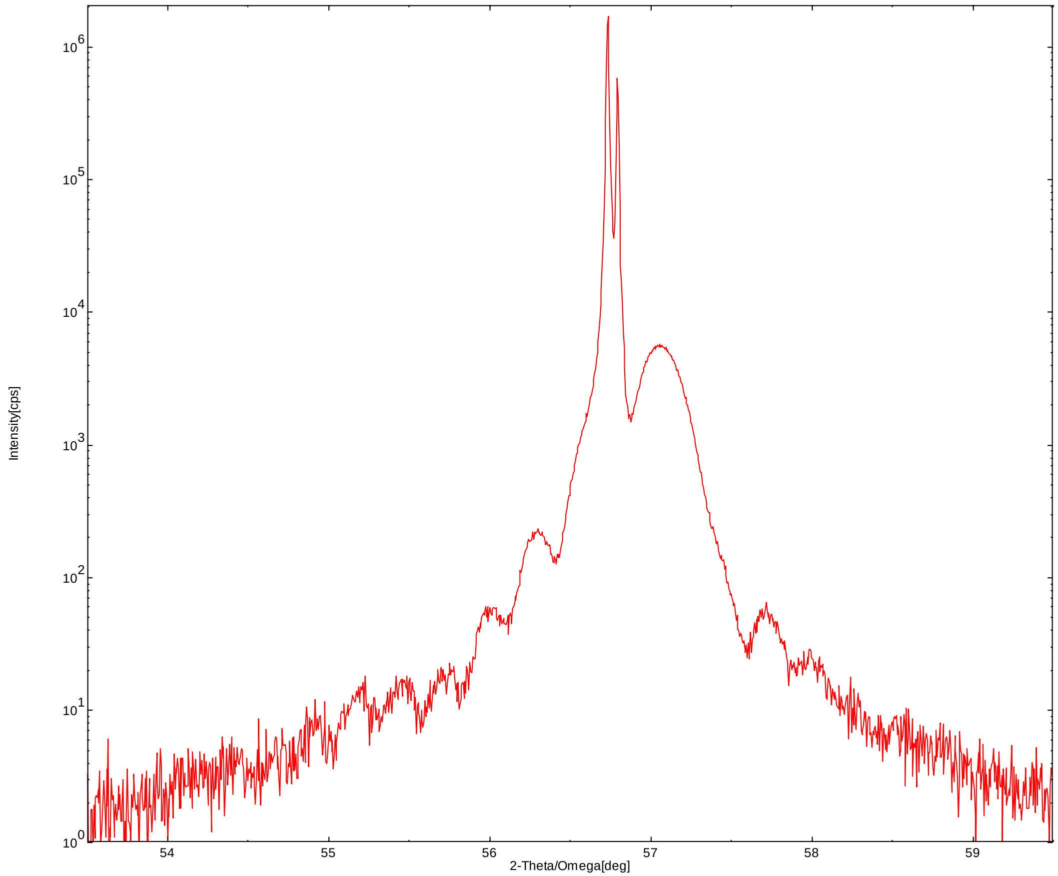
Parallel beam for XRR – HyPix3000 0D

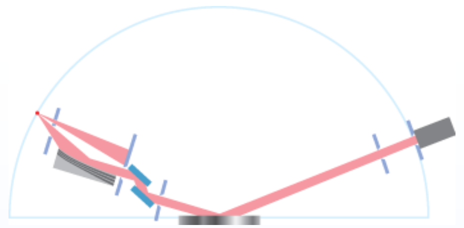


#		Thickness [nm]	Density [g/cm³]	Roughness [nm]
3	CdTe (surface layer)	1.239(8)	5.121(18)	0.246(3)
2	CdTe	**9.71(3)**	6.053 [fixed]	0
1	$Cd_{1-x}Mg_xTe$	**27.41(4)**	5.50(4)	0.34(3)
0	CdTe (thick layer)	0.0 [fixed]	6.053 [fixed]	0.40(3)

2359 / InSb (004) RC raw data

Ge(220)x2 – HyPix3000 0D



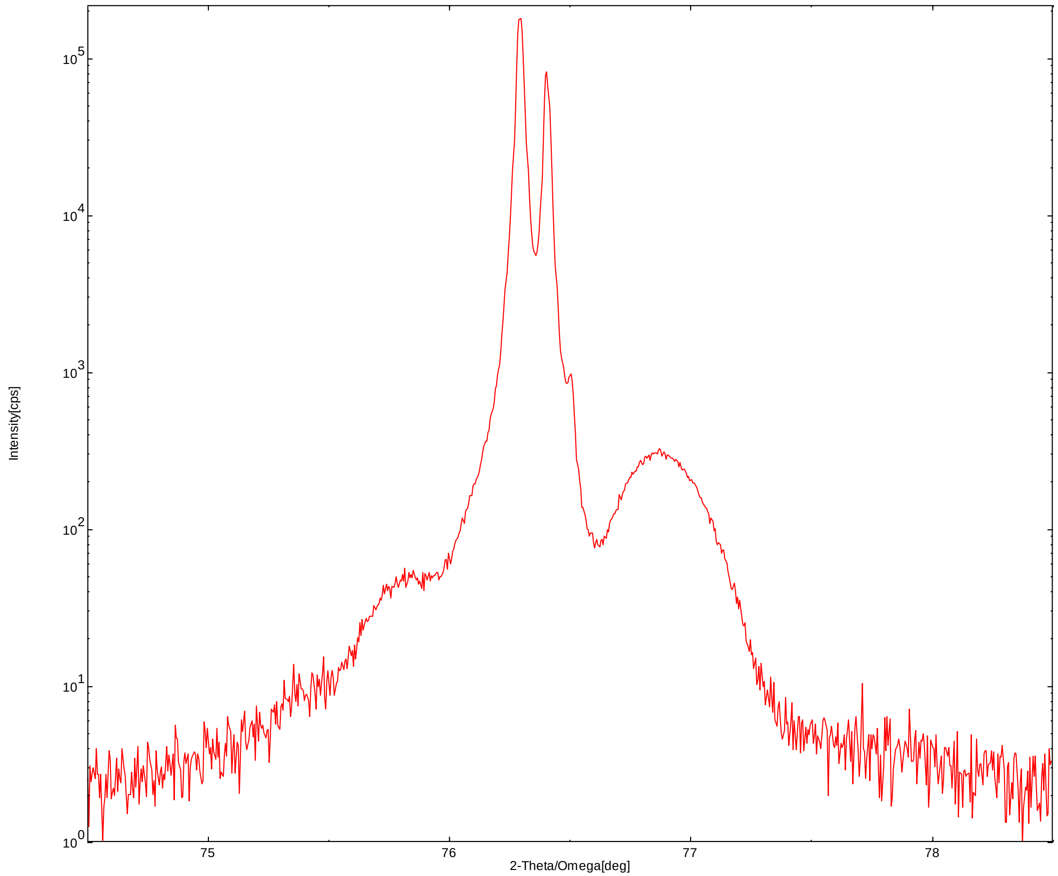


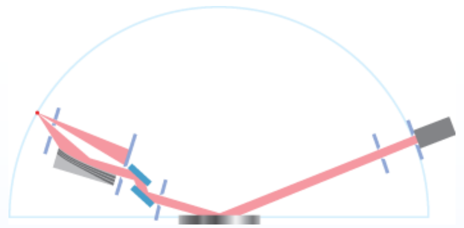
SmartLab / Standard
PB + Ge(220)x2

Att.:	χ-φ attachment
Detector:	HyPix3000 0D
XG:	40 kV – 44 mA
SI:	1.0 x 5 mm
Soller S.:	5 º
RS1:	1.0 mm
RS2:	1.0 mm
$2\theta / \omega$:	53.5 º – 59.5 º
	0.005 º step
Speed:	0.12 º / min

2359 / InSb (115) RC raw data

Ge(220)x2 – HyPix3000 0D



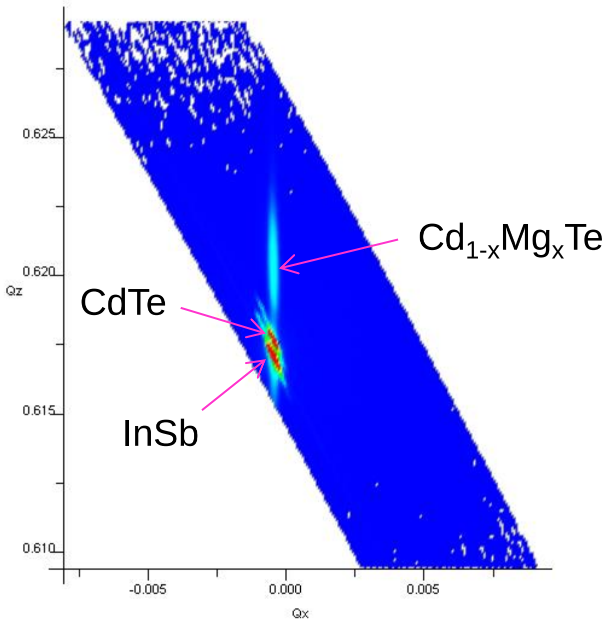


SmartLab / Standard
PB + Ge(220)x2

Att.:	χ-φ attachment
Detector:	HyPix3000 0D
XG:	40 kV – 44 mA
SI:	1.0 x 5 mm
Soller S.:	5 º
RS1:	1.0 mm
RS2:	1.0 mm
2θ / ω :	74.5 º – 78.5 º
	0.005 º step
Speed:	0.8 0º / min

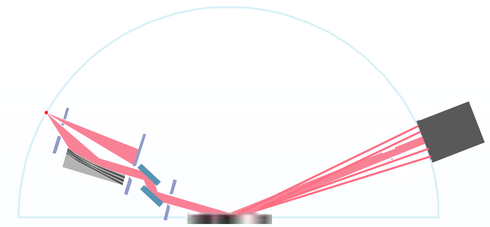
2359 / fast RSM InSb (004)

Ge(220)x2 – HyPix 3000 1D



Square root intensity scale

Name	*X*	*Y*	Δ*d/d*	Width(x)	Width(y)
InSb	-0.00044	0.617057	0.000%	0.000097	0.000196
CdTe	-0.00046	0.617695	-0.064%	0.000095	0.000195
Cd$_{1-x}$Mg$_x$Te	-0.00044	0.620244	-0.319%	0.000270	0.001976

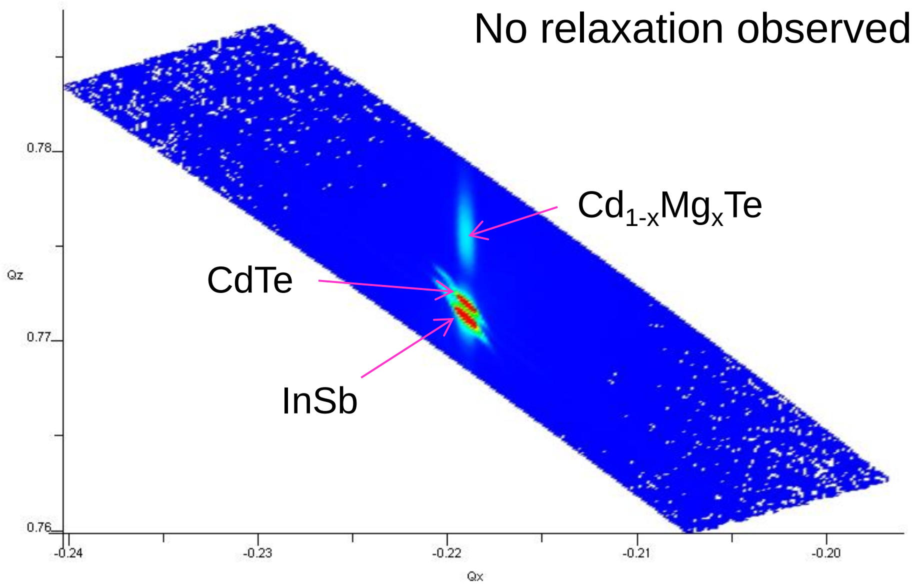


SmartLab / Standard
PB + Ge(220)x2

Att.:	χ-φ attachment
Detector:	HyPix3000 1D
XG:	40 kV – 44 mA
SI:	0.2 x 5 mm
Soller S.:	5 º
RS1:	1.0 mm
RS2:	1.0 mm
Axis:	ω step - 2θ scan
ω:	-0.1 º - + 0.5 º
	0.01 º step
2θ:	56.0 – 58.0 º
	0.008 º step
Speed:	10.0 º / min

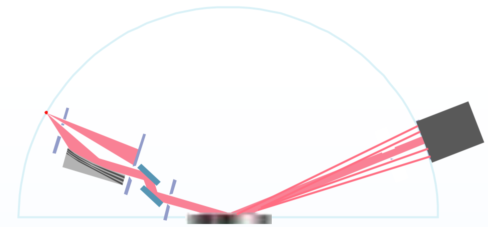
2359 / fast RSM InSb (115)

Ge(220)x2 – HyPix 3000 1D



Square root intensity scale

Name	*X*	*Y*	*Δd/d*	Width(x)	Width(y)
InSb	-0.21899	0.771151	0.000%	0.000265	0.000221
CdTe	-0.21906	0.772020	-0.087%	0.000207	0.000167
$Cd_{1-x}Mg_xTe$	-0.21906	0.775655	-0.450%		



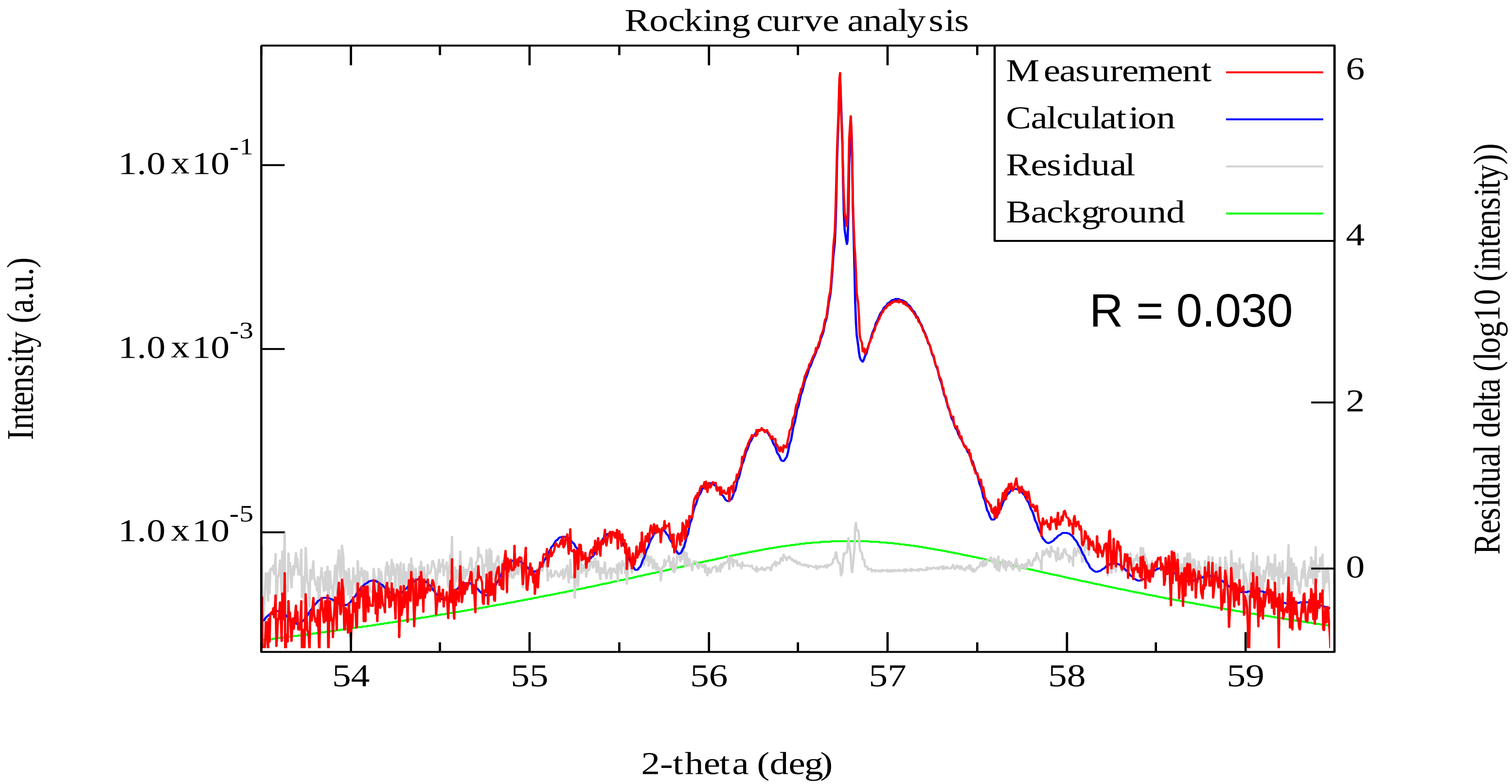
SmartLab / Standard
PB + Ge(220)x2

Att.:	χ-φ attachment
Detector:	HyPix3000 1D
XG:	40 kV – 44 mA
SI:	0.2 x 5 mm
Soller S.:	5 º
RS1:	1.0 mm
RS2:	1.0 mm
Axis:	*ω* step - 2*θ* scan
ω:	-0.2 º - + 0.6 º
	0.01 º step
2*θ*:	75.5 – 77.5 º
	0.008 º step
Speed:	10.0 º / min

Rigaku

2359 / InSb (004) RC analysis

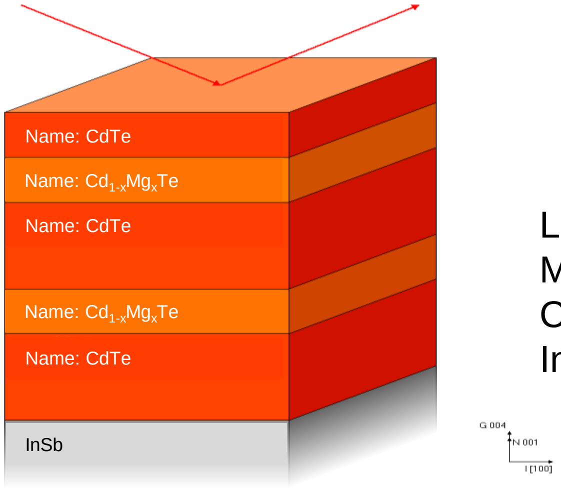
Ge(220)x2 – HyPix3000 0D



Rigaku

2359 / analysis results

Ge(220)x2 – HyPix3000 0D



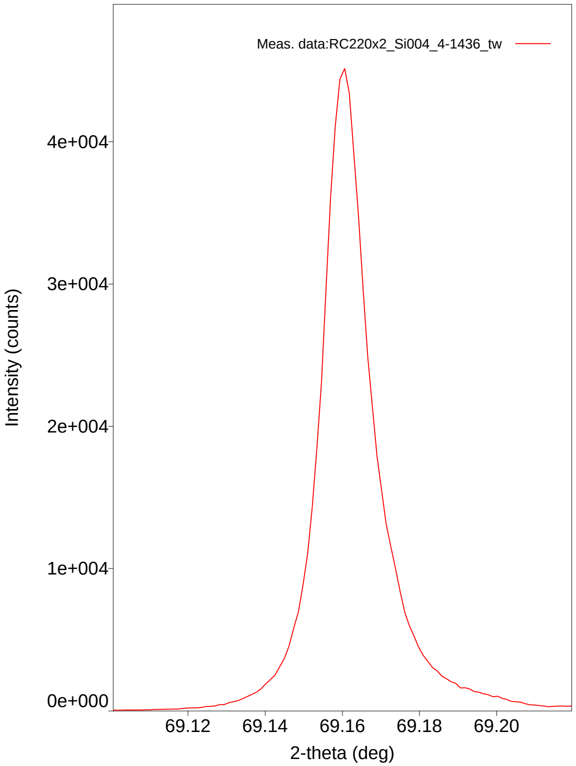
Lattice constants used for the analysis
MgTe a = 6.42 Å
CdTe a = 6.4823 Å (adjusted)
InSb a = 6.1794 Å

No.	Name	Diffraction hkl	Relax [%]	Thickness [nm]	MgTe ratio, x
5	CdTe	0 0 4	0	9.66(6)	
4	$Cd_{1-x}Mg_xTe$	0 0 4	0	27.56(7)	0.3319(17)
3	CdTe	0 0 4	0	1000 [fixed]	
2	$Cd_{1-x}Mg_xTe$	0 0 4	0	33.1(4)	0.274(3)
1	CdTe	0 0 4	0	1000 [fixed]	
0	InSb	0 0 4	N/A	N/A	N/A

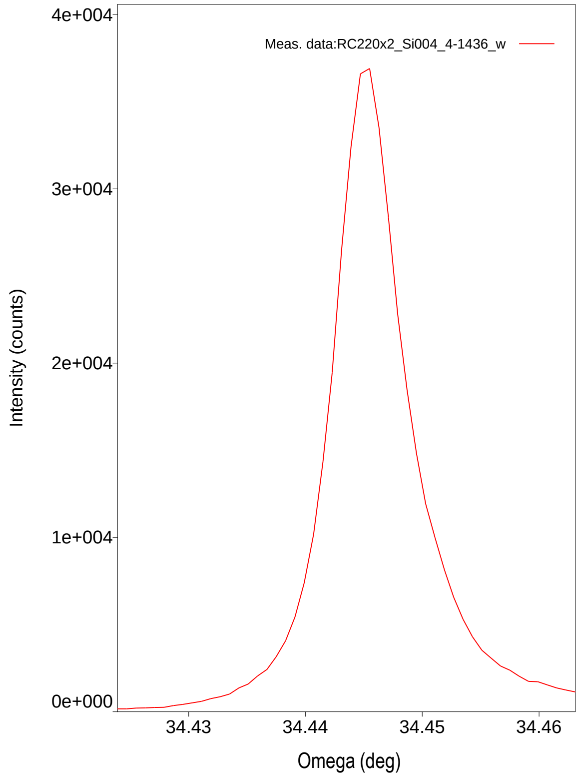
4-1436 / Si(004) RC raw data

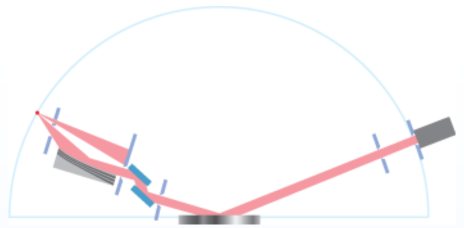
Ge(220)x2 – HyPix3000 0D

Si(004) 2θ/ω



Si(004) ω, Δω = 0.0136º



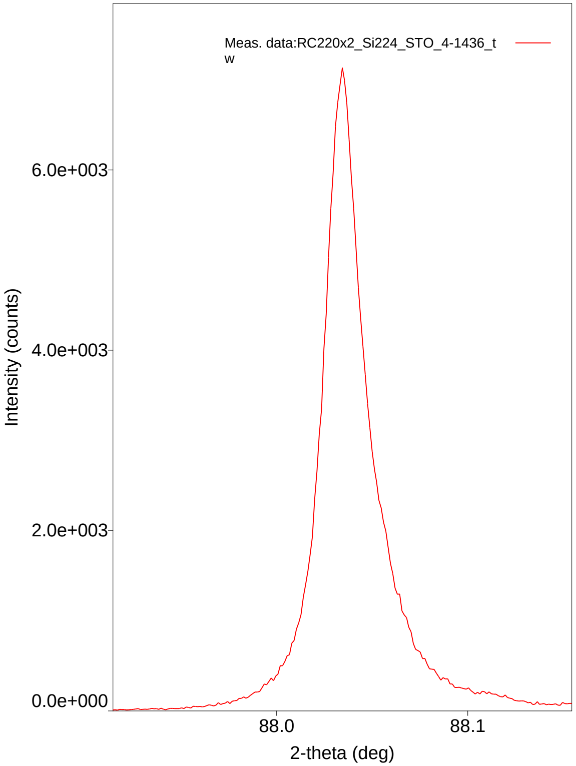


SmartLab / Standard	
PB + Ge(220)x2	
Att.:	χ-φ attachment
Detector:	HyPix3000 0D
XG:	40 kV – 44 mA
SI:	1.0 x 10 mm
Soller S.:	5 º
RS1:	1.0 mm
RS2:	1.0 mm
2θ / ω :	+/- 0.06 º
	0.0012 º step
Speed:	1 º / min
ω :	+/- 0.02 º
	0.0008 º step
Speed:	0.8 º / min

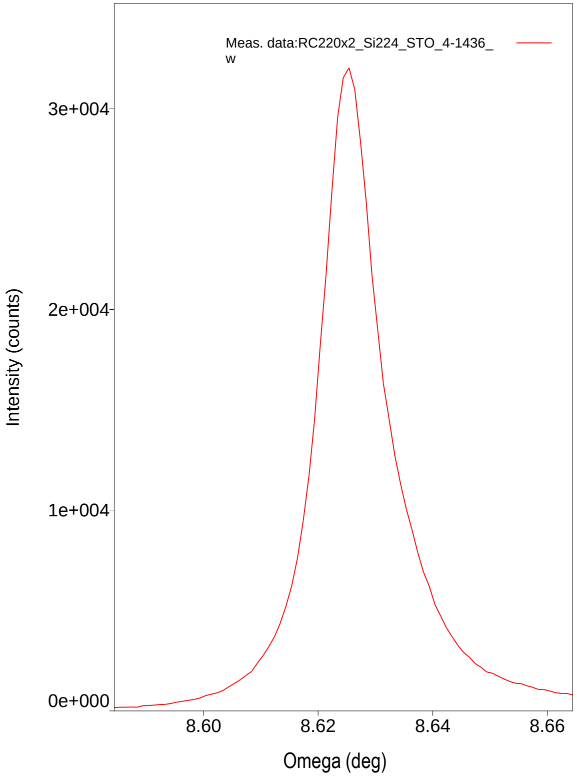
4-1436 / Si(224) RC raw data

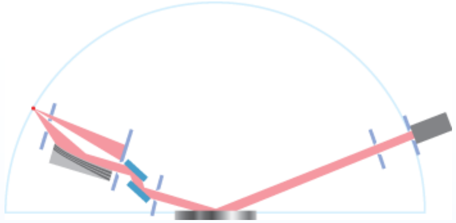
Ge(220)x2 – HyPix3000 0D

Si(224) 2θ/ω



Si(224) ω, Δω = 0.0143º





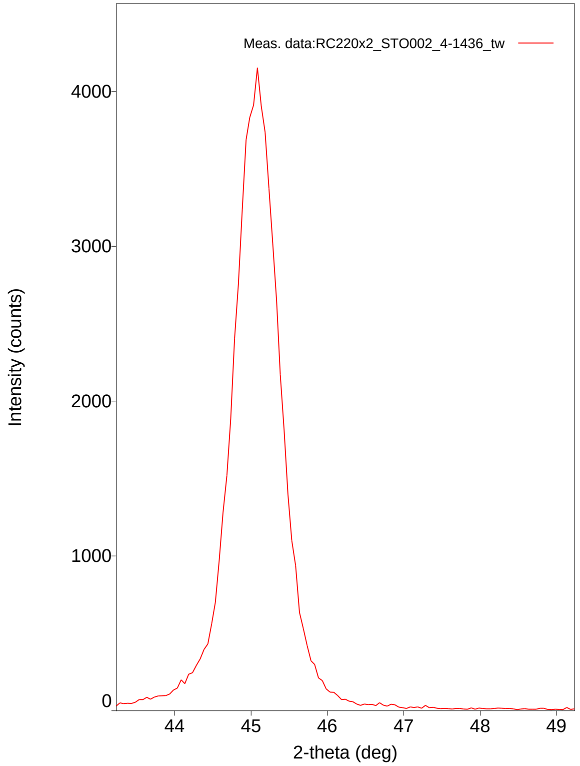
SmartLab / Standard
PB + Ge(220)x2

Att.:	χ-φ attachment
Detector:	HyPix3000 0D
XG:	40 kV – 44 mA
SI:	1.0 x 10 mm
Soller S.:	5 º
RS1:	1.0 mm
RS2:	1.0 mm
2θ / ω :	+/- 0.06 º
	0.0012 º step
Speed:	1 º / min
ω :	+/- 0.02 º
	0.0008 º step
Speed:	0.8 º / min

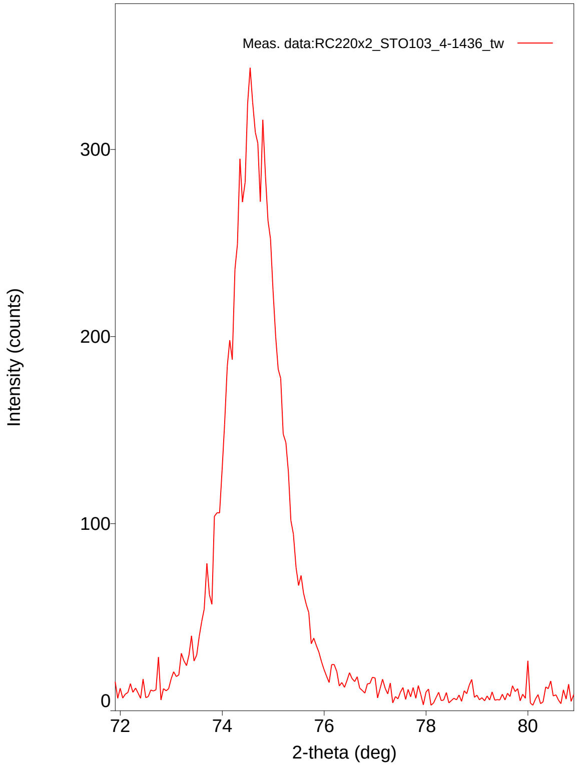
4-1436 / BTO(002)/(103) RC raw data

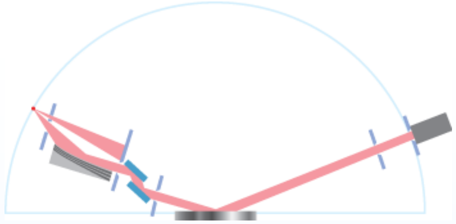
Ge(220)x2 – HyPix3000 0D

BTO(002) 2θ/ω



BTO(103) ω, Δω = 1.19º

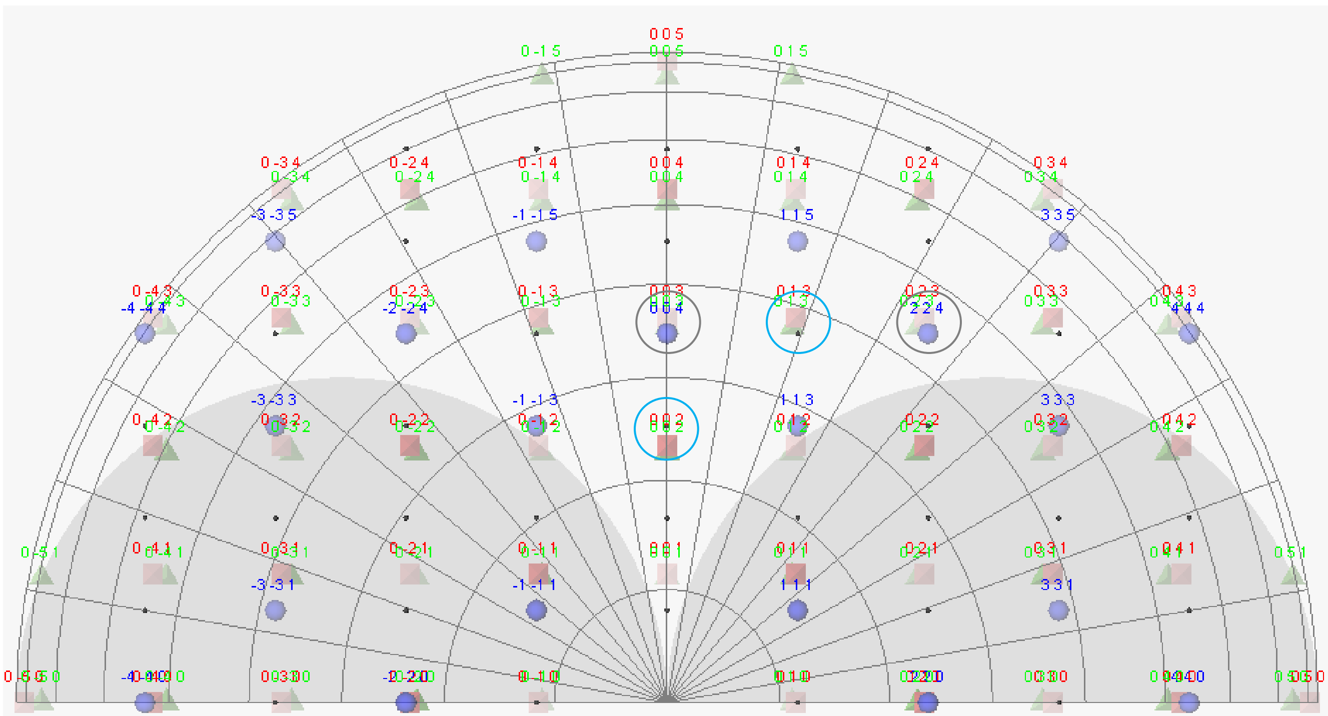




SmartLab / Standard	
PB + Ge(220)x2	
Att.:	χ-φ attachment
Detector:	HyPix3000 0D
XG:	40 kV – 44 mA
SI:	1.0 x 10 mm
Soller S.:	5 º
RS1:	1.0 mm
RS2:	1.0 mm
2θ / ω :	+/- 3.0 º (002)
	+/- 4.5 º (103)
	0.05 º step
Speed:	0.1 º / min

Rigaku

BTO/STO/Si reciprocal space simulation



- Si(single)(Sub)
- SrTiO3(L1)
- BaTiO3(cub)(L2)

○ Measured reflections

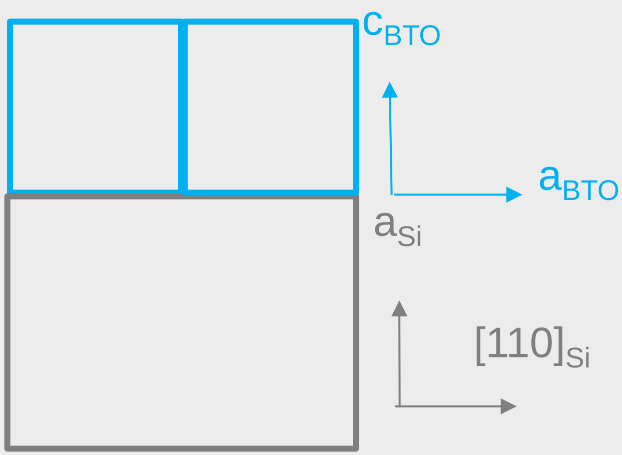
Rigaku

4-1436 / BTO analysis

Ge(220)x2 – HyPix3000 0D

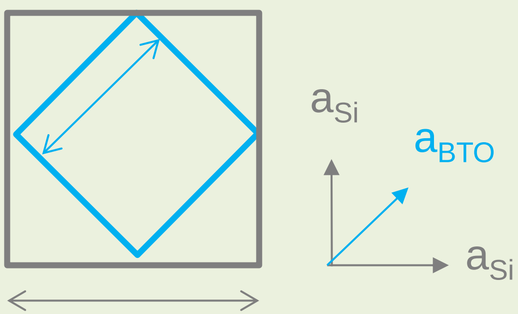
	Diffraction angle [deg]		Lattice constant [Å]	
#	(0 0 2)	(1 0 3)	c	a
4-1436	45.053	74.6	4.024	3.996

Side view



Top view

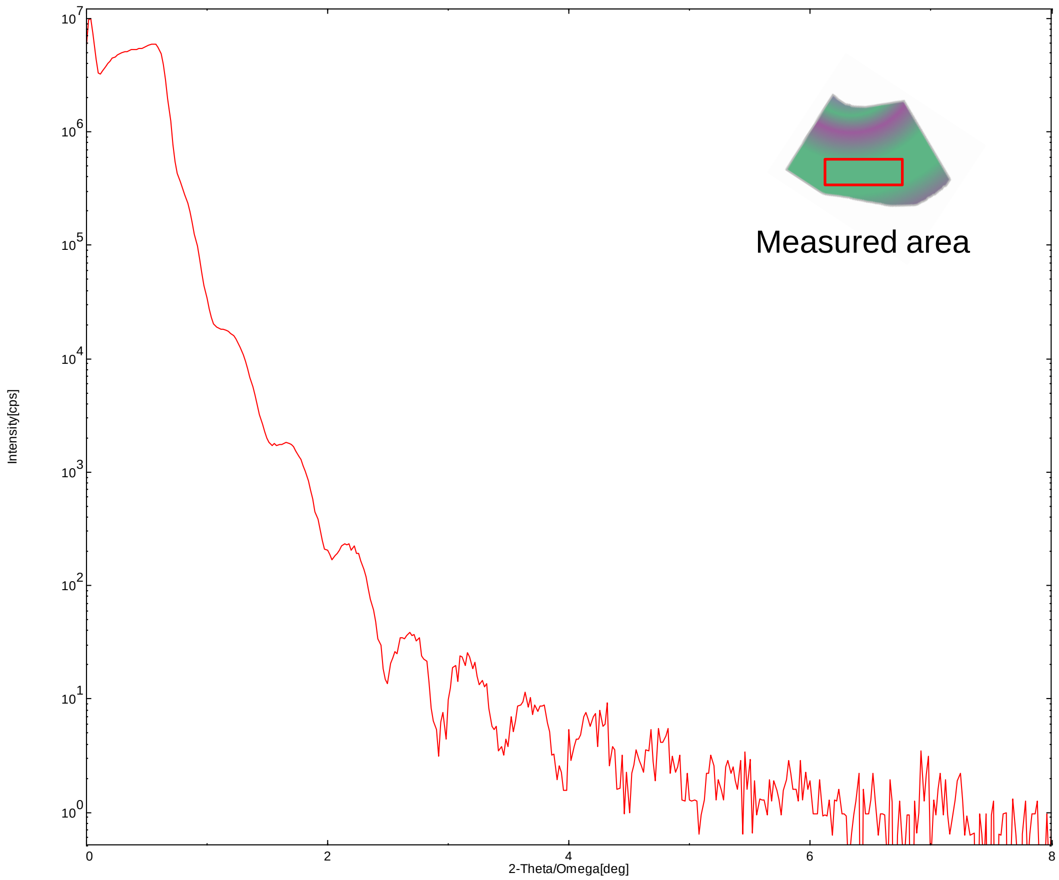
Lattice matching
BTO a = 3.840 Å

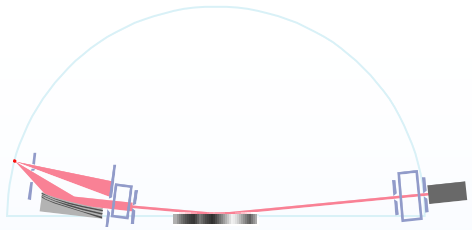


Si a = 5.431 Å

GaN HEMT / reflectivity raw data

Parallel beam for XRR – HyPix3000 0D



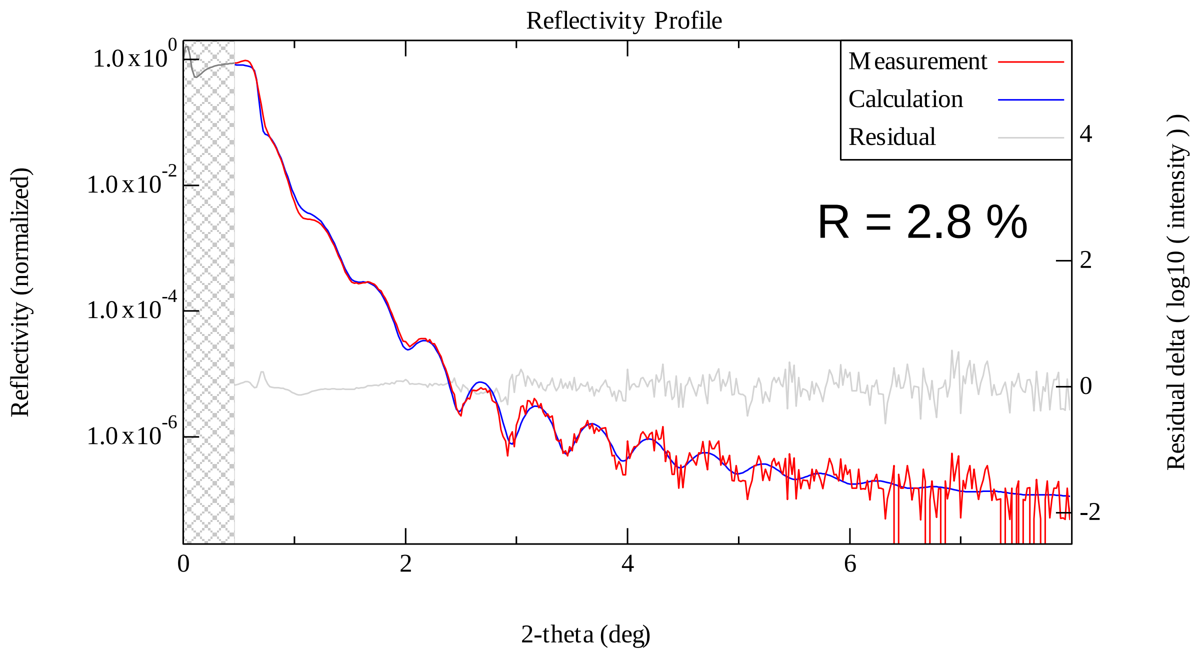


SmartLab / Standard
Parallel beam

Att.:	Standard
Detector:	HyPix3000 0D
XG:	40 kV – 44 mA
SI:	0.1 x 5 mm
Soller S.:	5 º
RS1:	0.25 mm
RS2:	0.35 mm
Axis:	θ / 2θ scan
Range:	0.0 – 8.0 º
Step:	0.02 º
Speed:	0.4 º / min

GaN HEMT / reflectivity analysis

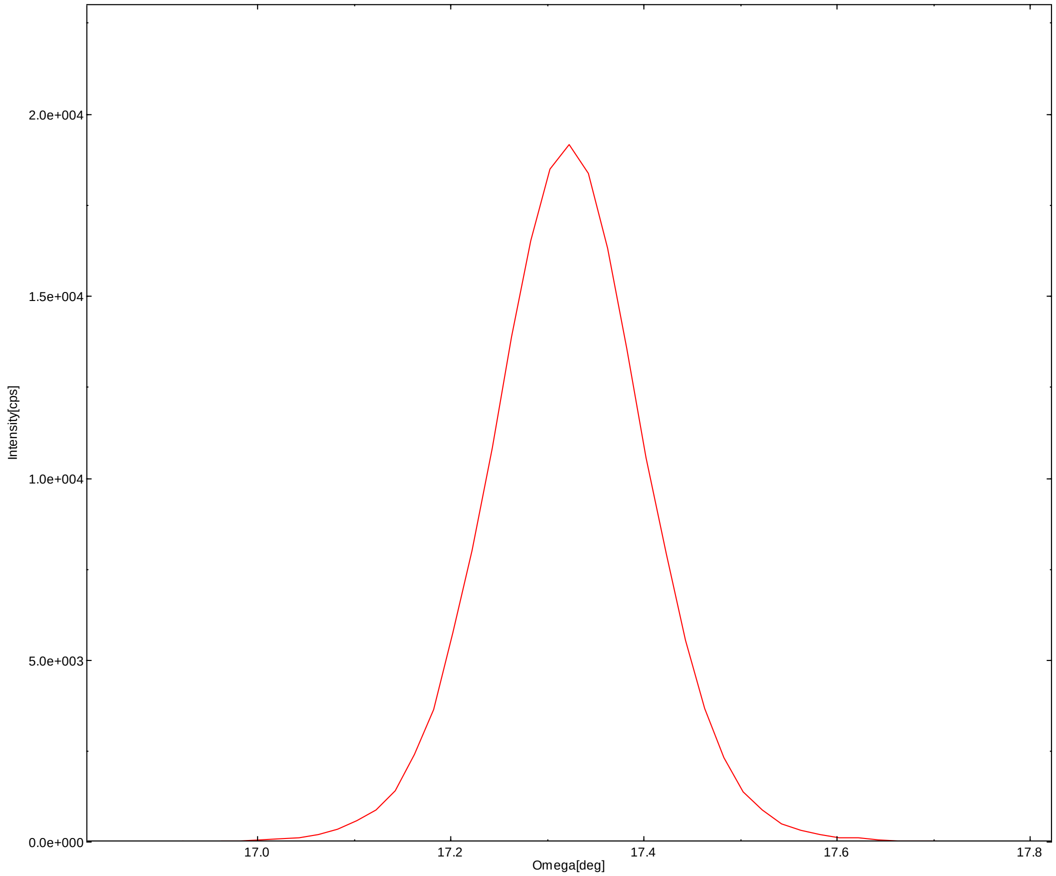
Parallel beam for XRR – HyPix3000 0D

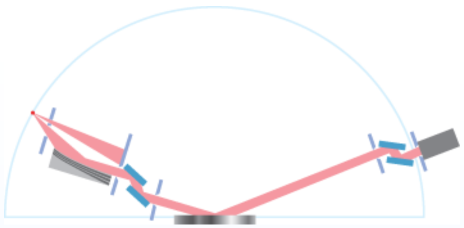


#		Thickness [nm]	Density [g/cm³]	Roughness [nm]
2	AlGaN (surface layer)	0.87(10)	0.73(8)	0.0(8)
1	AlGaN	**16.12(9)**	5.36(5)	1.25(4)
0	GaN (thick layer)	N/A	6.08646 [fixed]	0.46(4)

GaN HEMT / GaN (002) ω scan raw data

Ge(220)x2 – Ge(220)x2 – HyPix3000 0D



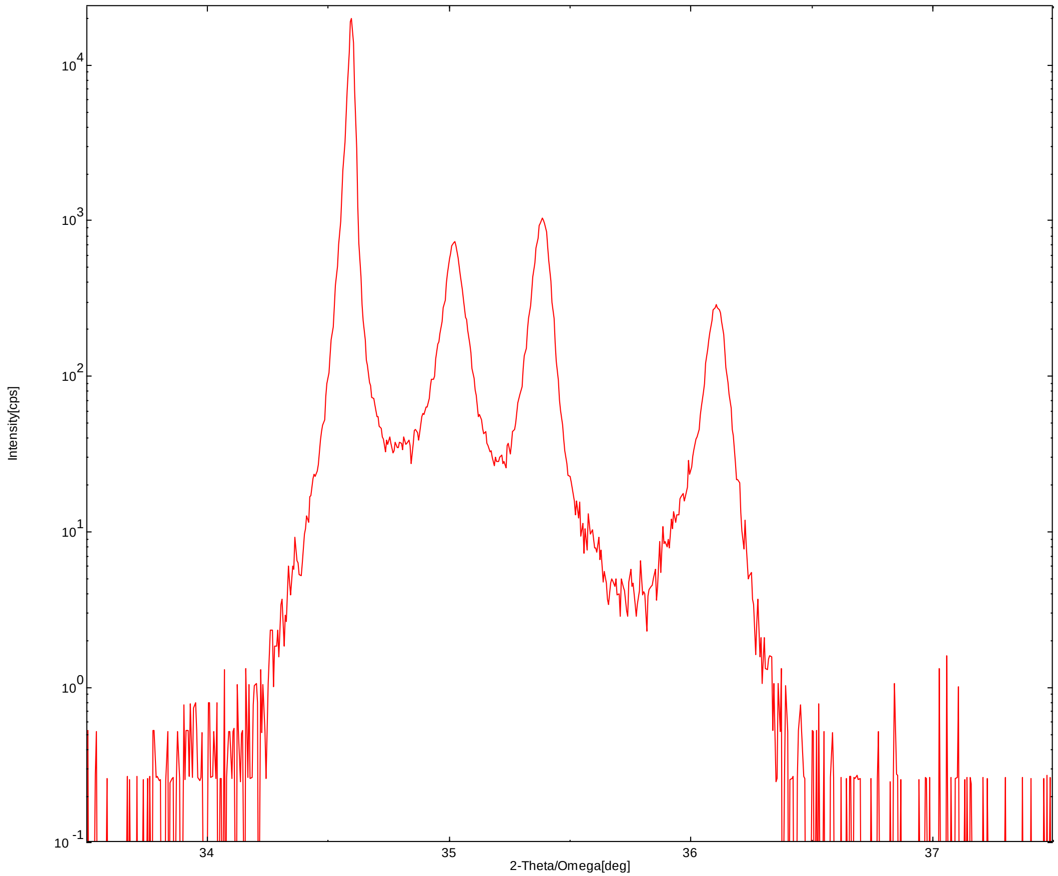


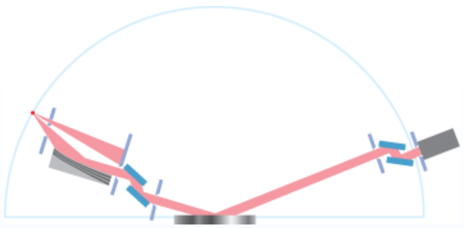
SmartLab / Standard
PB + Ge(220)x2-Ge(220)x2

Att.:	χ-φ attachment
Detector:	HyPix3000 0D
XG:	40 kV – 44 mA
SI:	1.0 x 5 mm
Soller S.:	5 º
RS1:	1.0 mm
RS2:	1.0 mm
ω :	17.3177 º +/- 0.5 º
	0.02 º step
Speed:	1.0 º / min

GaN HEMT / GaN (002) RC raw data

Ge(220)x2 – Ge(220)x2 – HyPix3000 0D





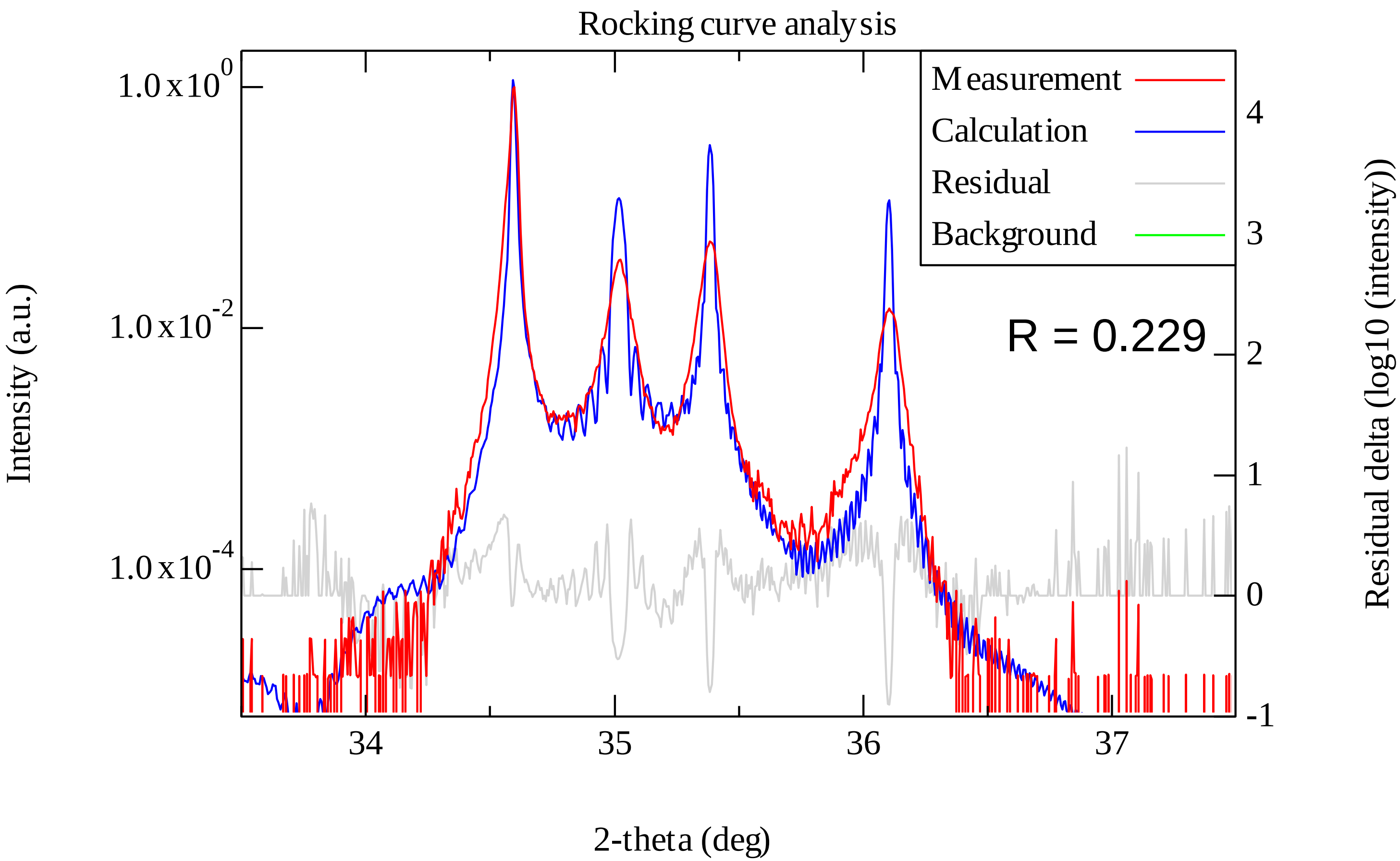
SmartLab / Standard

PB + Ge(220)x2-Ge(220)x2

Att.:	χ-φ attachment
Detector:	HyPix3000 0D
XG:	40 kV – 44 mA
SI:	1.0 x 5 mm
Soller S.:	5 º
RS1:	1.0 mm
RS2:	1.0 mm
$2\theta / \omega$:	33.5 º – 37.5 º
	0.006 º step
Speed:	0.1 º / min

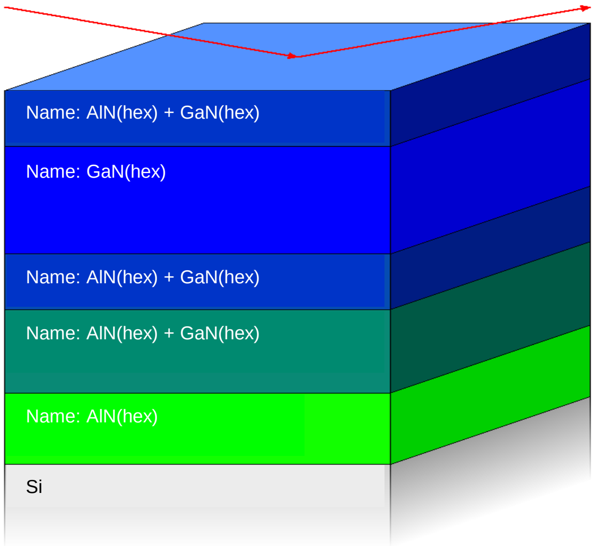
GaN HEMT / GaN (002) RC analysis

Ge(220)x2 – Ge(220)x2 – HyPix3000 0D



GaN HEMT / analysis results

Ge(220)x2 – Ge(220)x2 – HyPix3000 0D

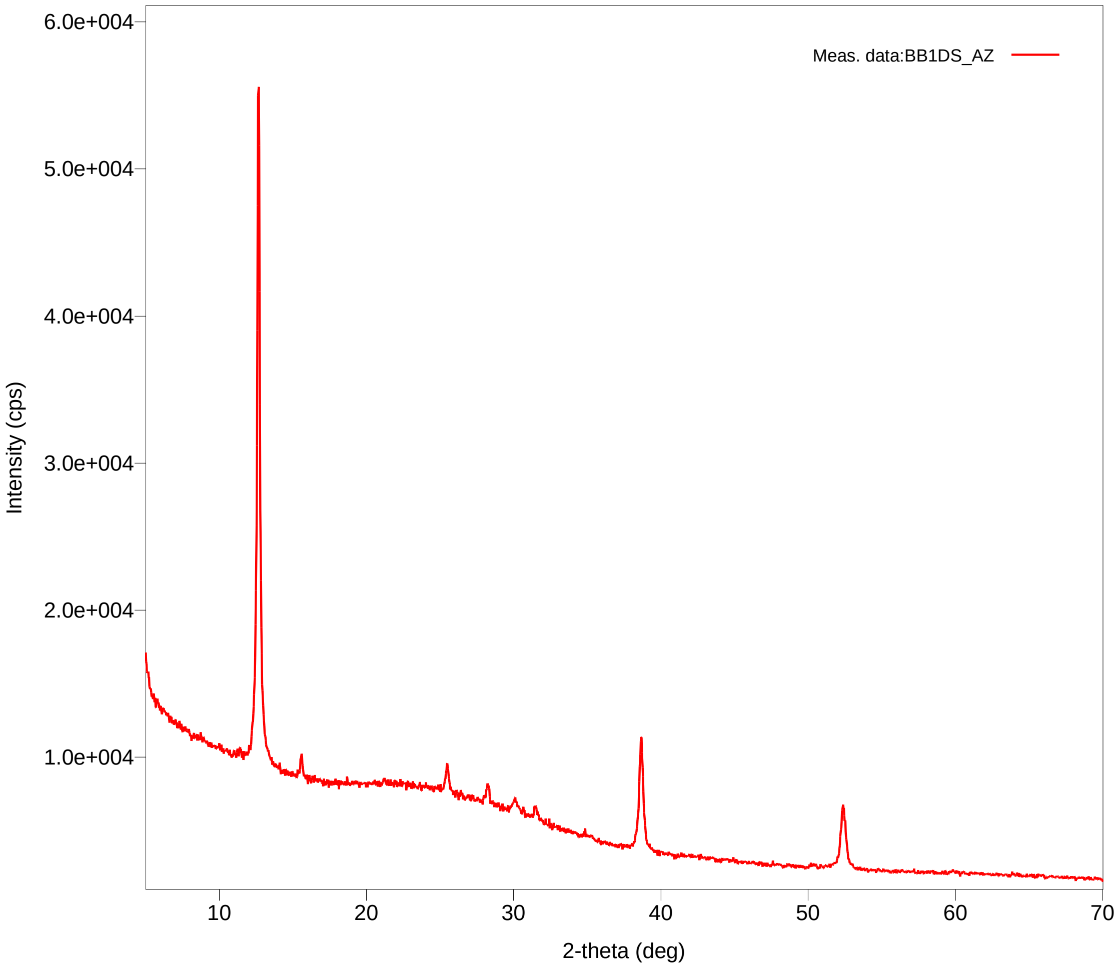


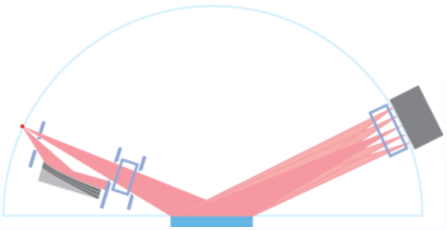
Lattice constants used for the analysis
AlN c = 4.9750 Å
GaN c = 5.1855 Å

No.	Name	Diffraction hkl	Relax [%]	Thickness [nm]	AlN ratio, x
5	$Al_xGa_{(1-x)}N$	0 0 2	0	16.12 [fixed]	0.26 [fixed]
4	GaN	0 0 2	750	750 [fixed]	N/A
3	$Al_xGa_{(1-x)}N$	0 0 2	200	200 [fixed]	0.29
2	$Al_xGa_{(1-x)}N$	0 0 2	450	450 [fixed]	0.535
1	AlN	0 0 2	400	400 [fixed]	N/A
0	Si	N/A	N/A	N/A	N/A

AZ / raw data

Bragg-Brentano focusing – HyPix3000 1D



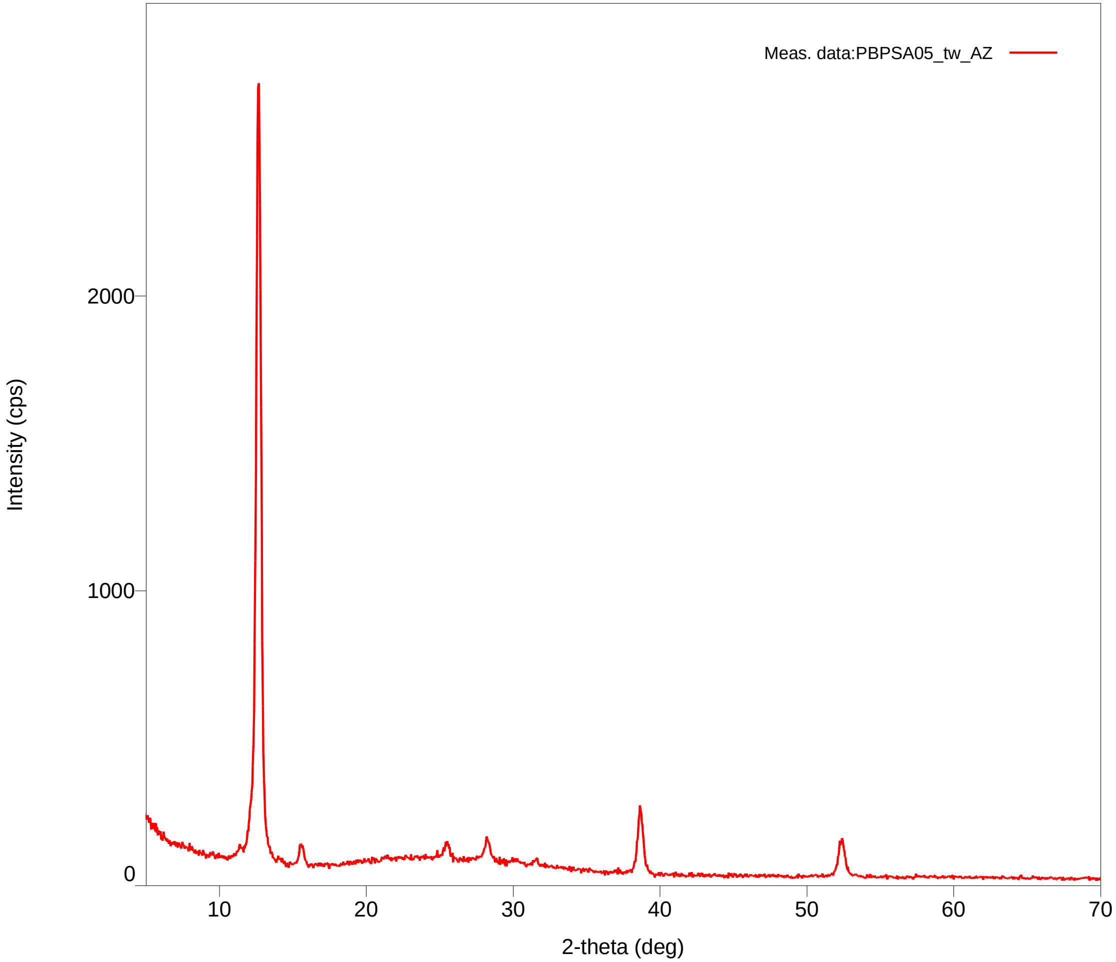


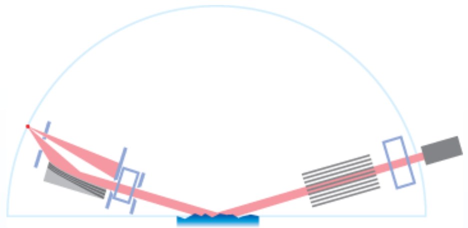
SmartLab / Standard
Bragg-Brentano

Att.:	Standard
Detector:	HyPix3000 1D
XG:	40 kV – 44 mA
SI:	2/3 º x 5 mm
RS1:	8 º
RS2:	20 mm
Soller S.:	5 º
Mono:	Kβ filter
Axis:	θ / 2θ scan
Range:	5.0 – 70.0 º
Step:	0.03 º
Speed:	6.0 º / min

AZ / raw data

PB/PSA out-of-plane – HyPix3000 0D



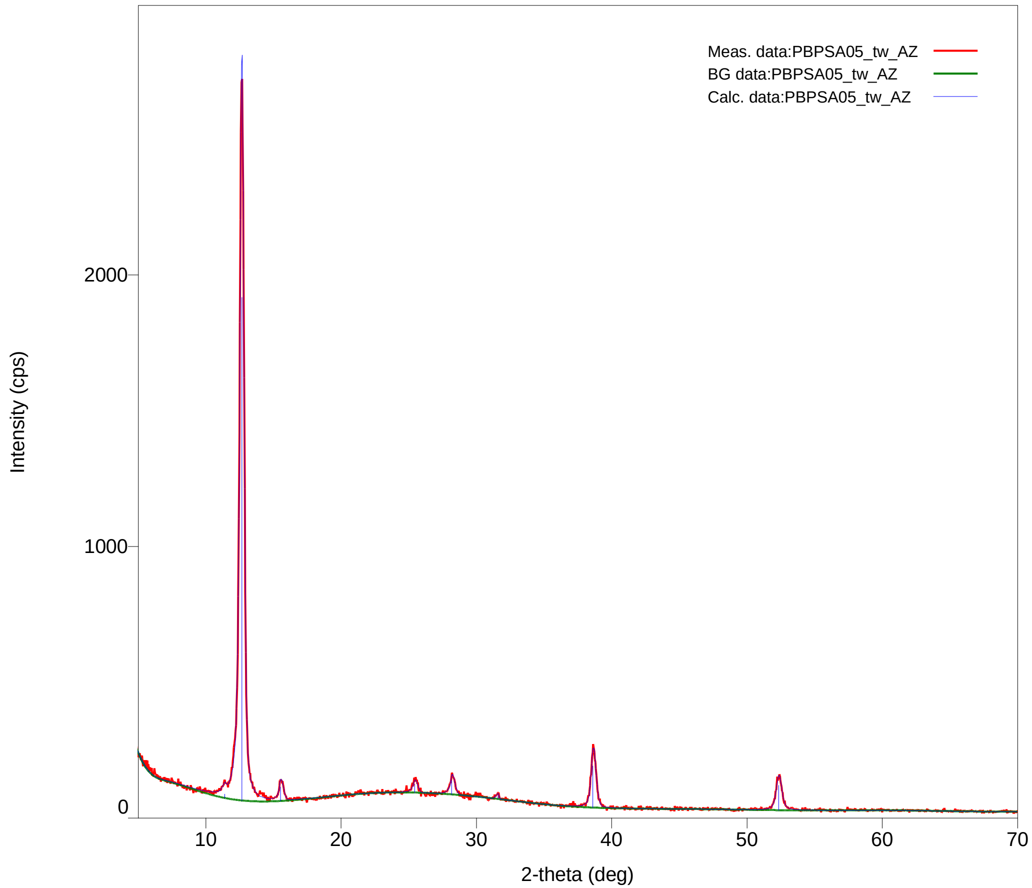


SmartLab / Standard
Parallel beam / PSA

Att.:	Standard
Detector:	HyPix3000 0D
XG:	40 kV – 44 mA
Sl:	1 x 5 mm
PSA:	0.5 º
Soller S.:	5 º
Mono:	none
Axis:	θ / 2θ scan
Range:	5.0 – 70.0 º
Step:	0.04 º
Speed:	1.0 º / min

AZ / peak search

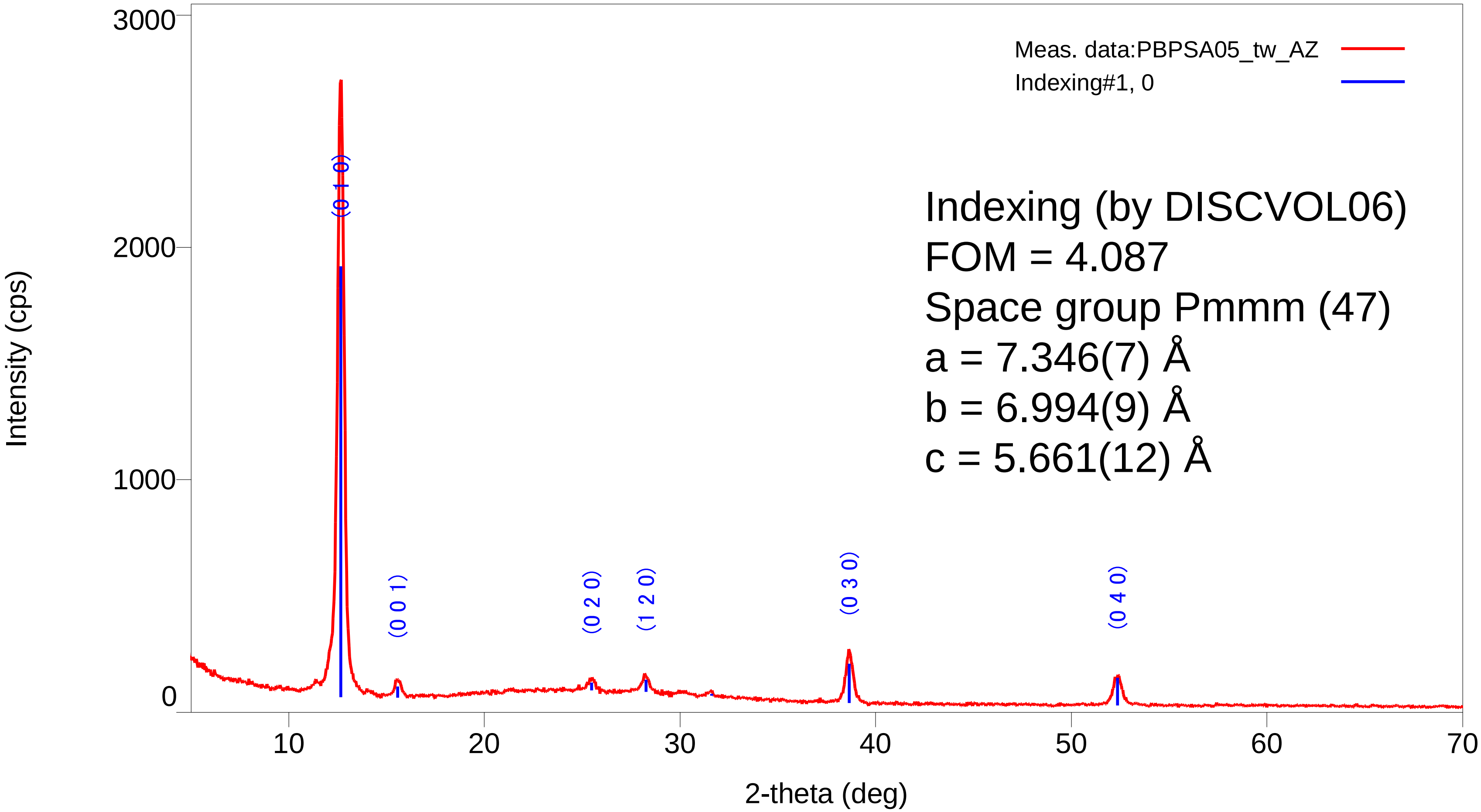
PB/PSA out-of-plane – HyPix3000 0D



	2-theta [deg]	d-value [A]	Intensity [cps]	FWHM [deg]
1	11.40(10)	7.76(7)	15(2)	0.31(9)
2	12.654(4)	6.990(2)	1854(28)	0.359(3)
3	15.53(3)	5.702(13)	52(5)	0.35(4)
4	25.44(7)	3.498(10)	32(4)	0.39(8)
5	28.164(15)	3.1659(17)	51(5)	0.36(4)
6	31.60(3)	2.829(3)	14(2)	0.26(8)
7	38.616(18)	2.3297(11)	154(8)	0.410(15)
8	52.34(3)	1.7467(10)	92(6)	0.45(3)

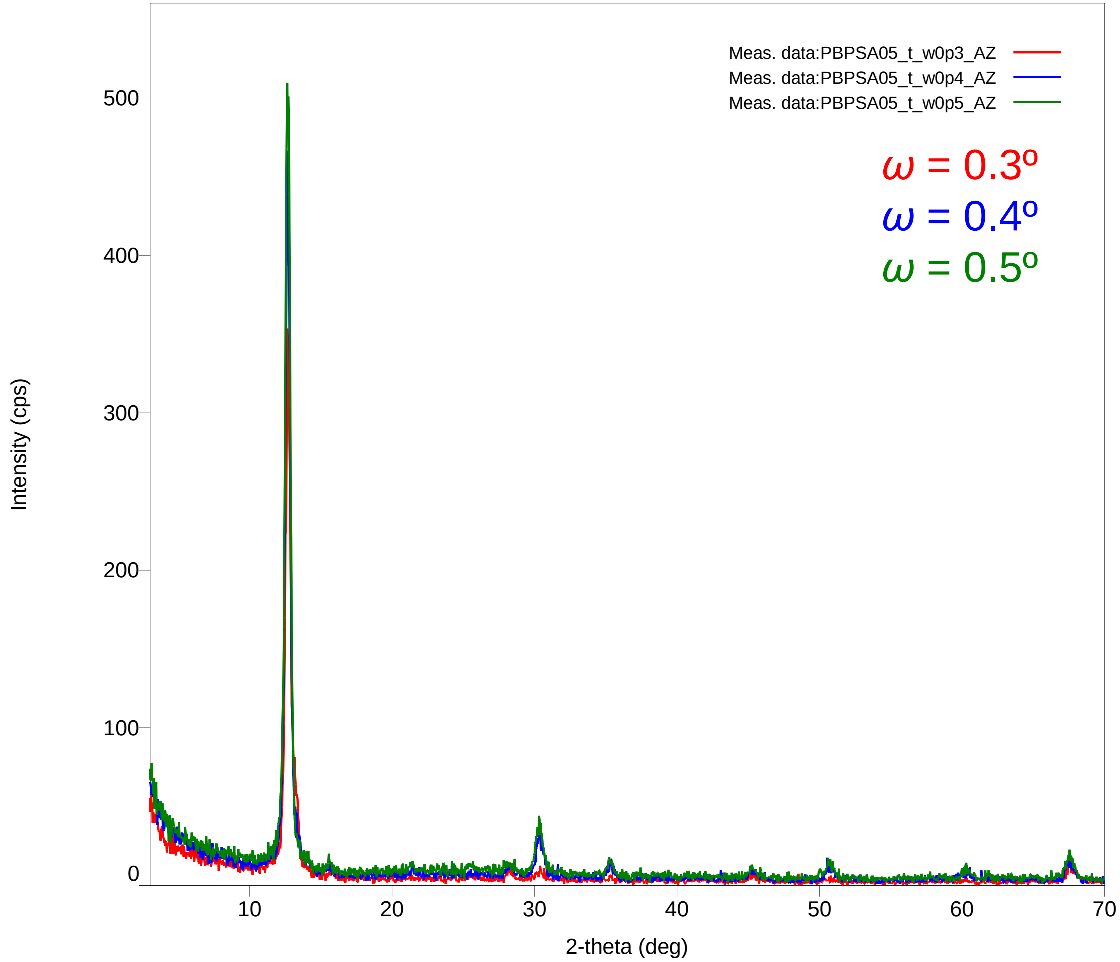
AZ / indexing

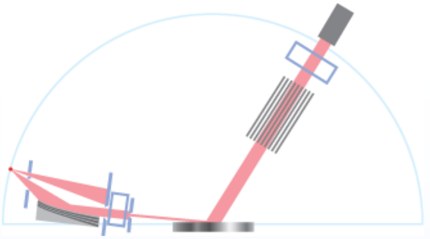
PB/PSA out-of-plane – HyPix3000 0D



AZ / raw data

PB/PSA GIXRD – HyPix3000 0D





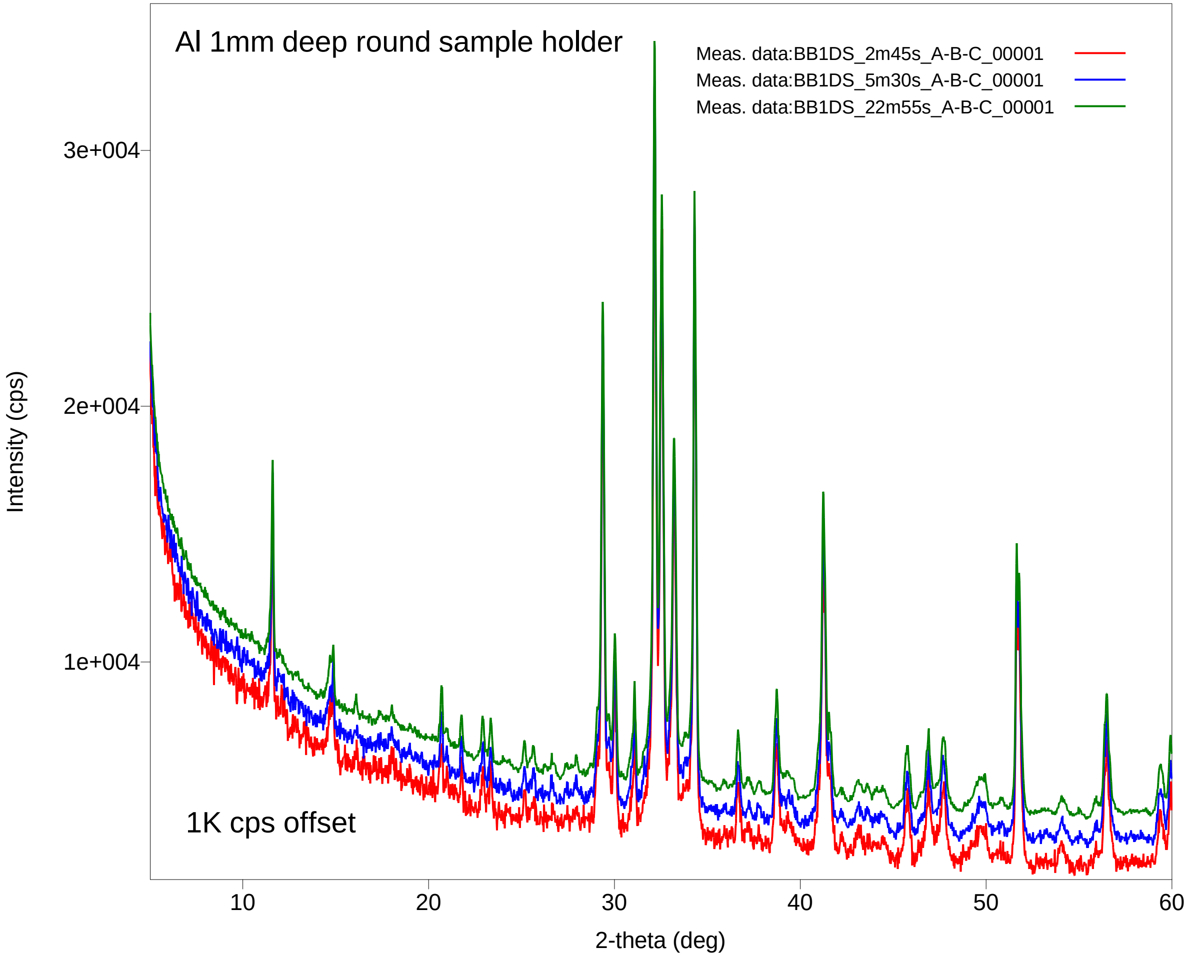
SmartLab / Standard
Parallel beam / PSA

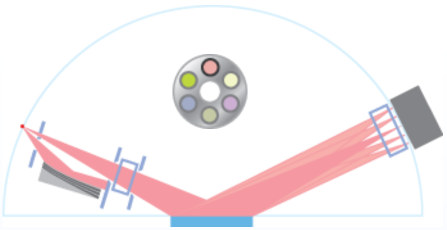
Att.:	Standard
Detector:	HyPix3000 0D
XG:	40 kV – 44 mA
SI:	0.07, 0.10, 0.12 x 5 mm
PSA:	0.5 º
Soller S.:	5 º
Mono:	none
Axis:	2θ scan
Range:	5.0 – 70.0 º
Step:	0.04 º
Speed:	1.0 º / min
ω:	0.3, 0.4, 0.5 º

Rigaku

A (cement) / raw data

Bragg-Brentano focusing – HyPix3000 1D





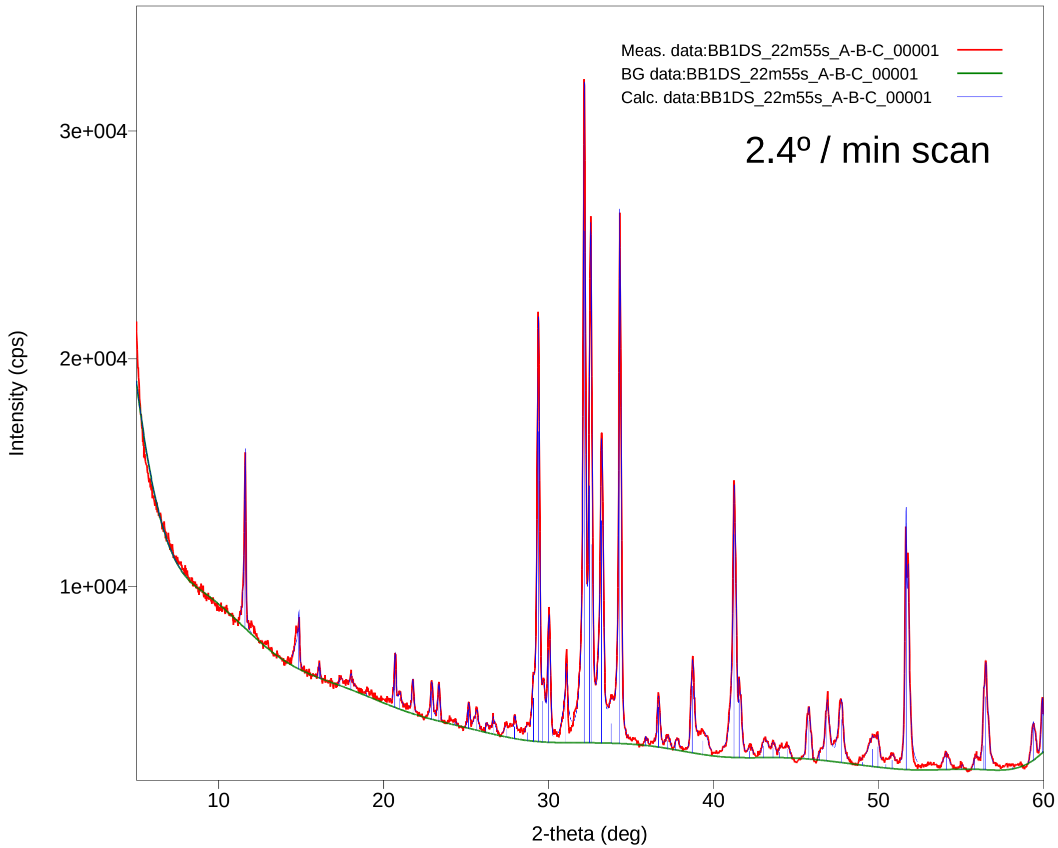
SmartLab / Standard
Bragg-Brentano

Att.:	ASC-6
Spin:	5 rpm
Detector:	HyPix3000 1D
XG:	40 kV – 44 mA
SI:	2/3 º
RS1:	8 º
RS2:	20 mm
Soller S.:	5 º
Mono:	Kβ filter
Axis:	θ / 2θ scan
Range:	5.0 – 60.0 º
Step:	0.02 º
Speed:	20, 10, 2.4 º / min

2.4º / min = 0.5 sec/point

A (cement) / peak search

Bragg-Brentano focusing – HyPix3000 1D

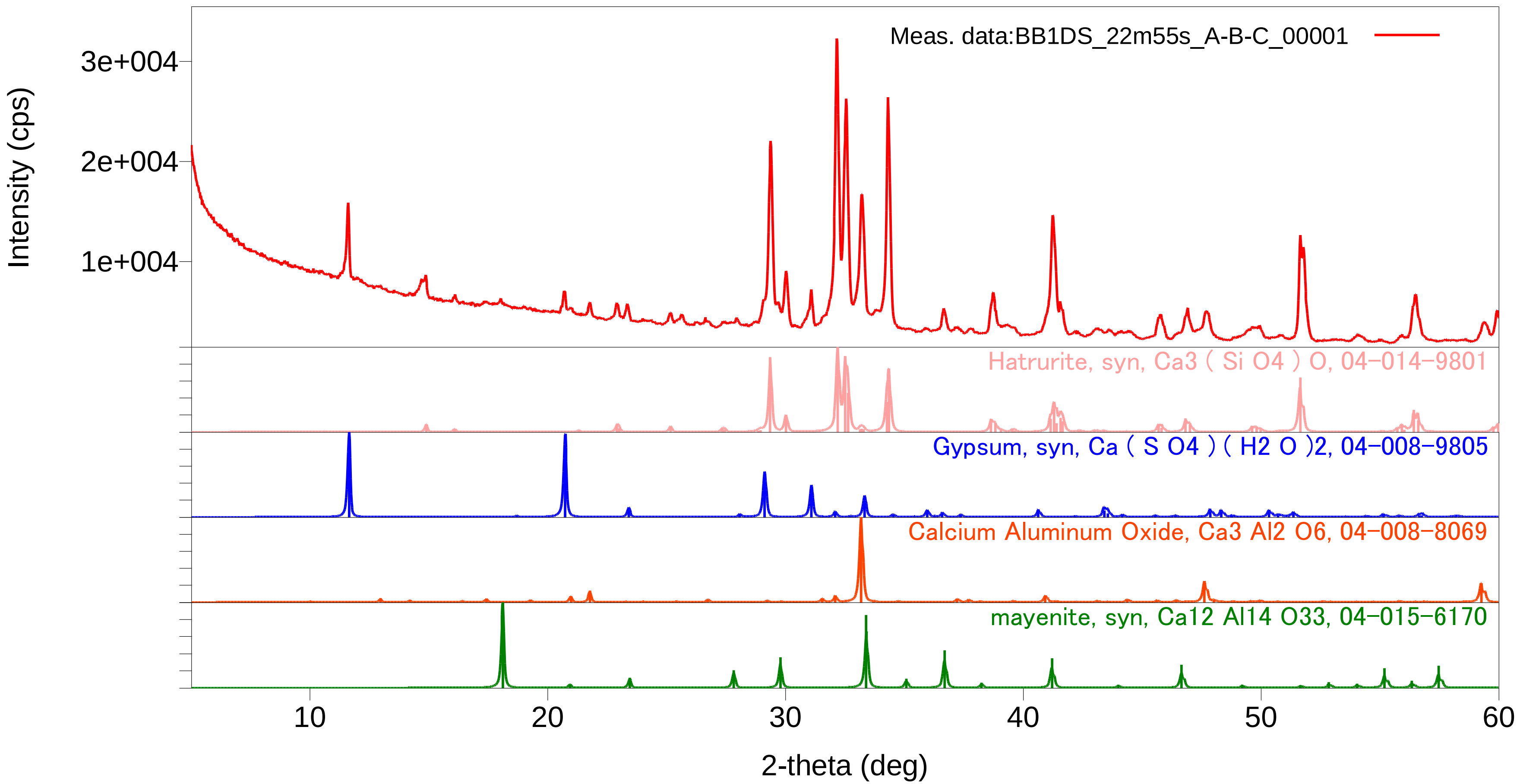


	2-theta [deg]	d-value [A]	Intensity [cps]	FWHM [deg]
1	11.592(6)	7.628(4)	5620(106)	0.098(6)
2	14.857(4)	5.9580(17)	1810(60)	0.150(11)
3	16.097(13)	5.502(4)	472(31)	0.102(15)
4	17.329(13)	5.113(4)	257(23)	0.29(9)
5	18.00(2)	4.924(5)	456(30)	0.16(4)
6	18.96(3)	4.678(8)	146(17)	0.59(16)
7	20.673(5)	4.2930(10)	1900(62)	0.098(10)
8	20.939(17)	4.239(3)	477(31)	0.17(4)
9	21.774(11)	4.078(2)	1128(48)	0.121(15)
10	22.879(9)	3.8838(14)	1222(50)	0.134(8)
11	23.336(10)	3.8088(16)	1218(50)	0.133(10)
12	24.32(6)	3.657(9)	143(17)	0.36(9)
13	25.148(12)	3.5383(16)	838(41)	0.141(14)
14	25.648(15)	3.471(2)	618(35)	0.25(2)
15	26.193(14)	3.3994(18)	370(27)	0.10(5)
16	26.628(12)	3.3449(15)	617(35)	0.12(3)
17	27.46(2)	3.245(3)	357(27)	1.11(11)
18	27.927(19)	3.192(2)	535(33)	0.09(2)
19	28.71(7)	3.107(7)	358(27)	0.3(3)
20	29.084(17)	3.0678(18)	1912(62)	0.22(6)

Total 61 peaks found

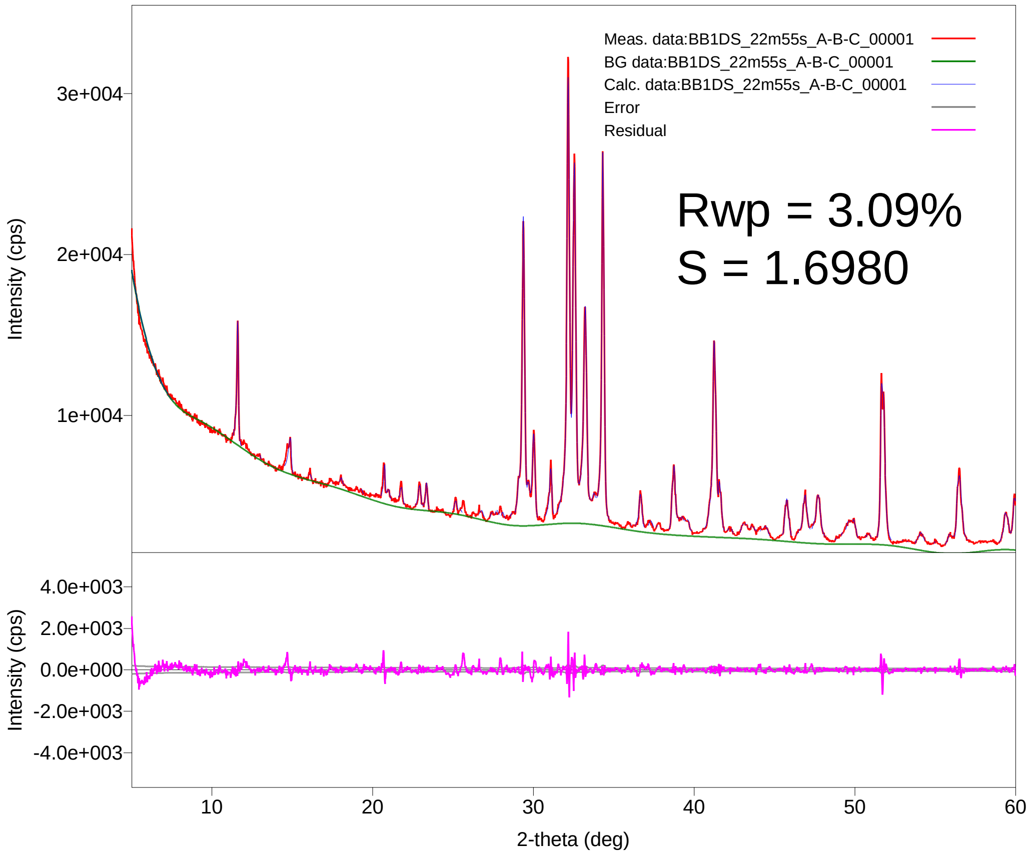
A (cement) / phase ID

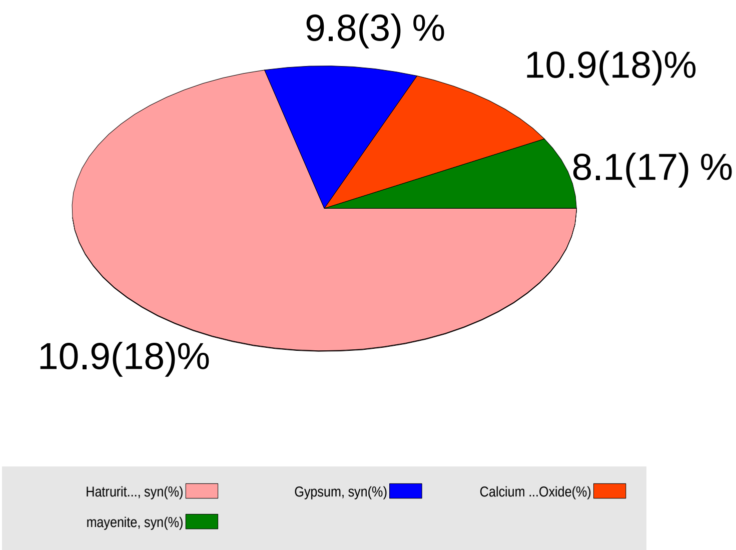
Bragg-Brentano focusing – HyPix3000 1D



A (cement) / WPPF

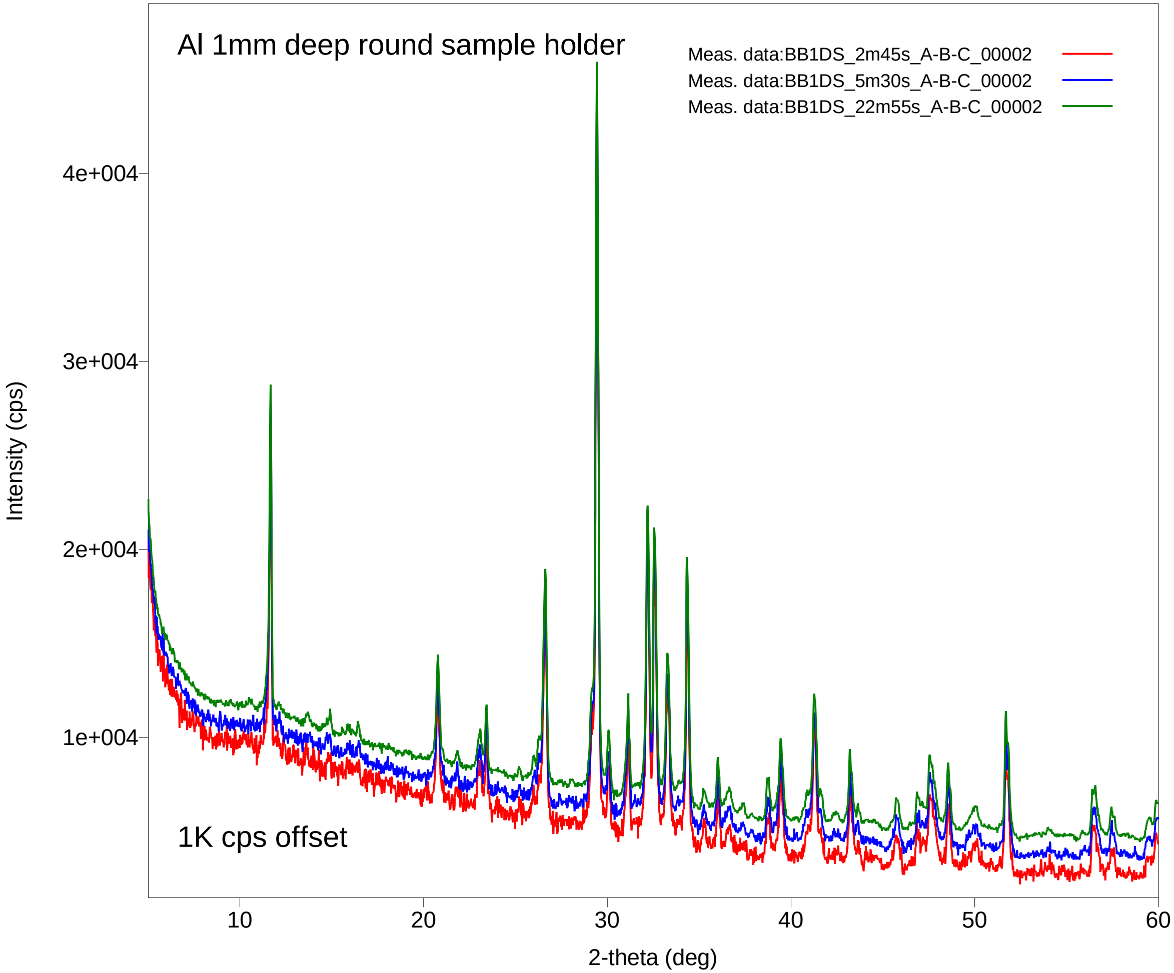
Bragg-Brentano focusing – HyPix3000 1D

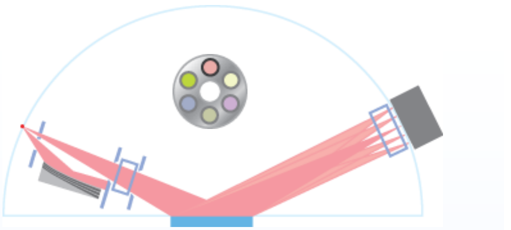




B (cement, fly ash) / raw data

Bragg-Brentano focusing – HyPix3000 1D





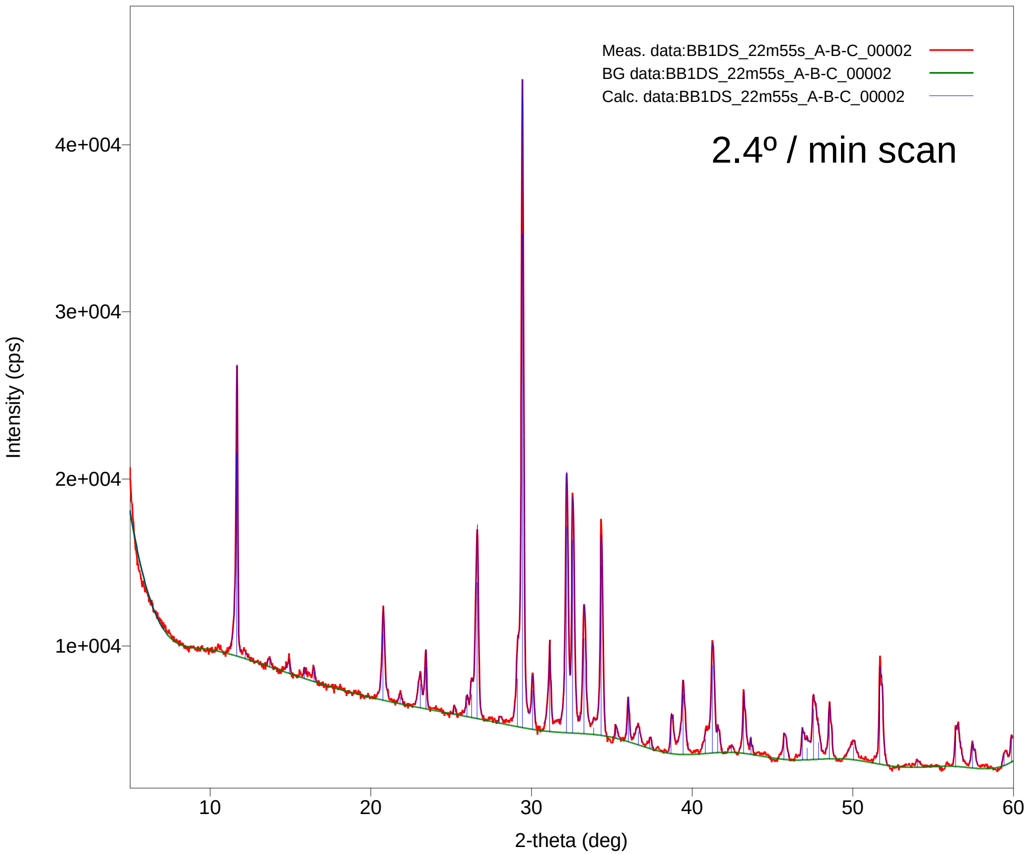
SmartLab / Standard
Bragg-Brentano

Att.:	ASC-6
Spin:	5 rpm
Detector:	HyPix3000 1D
XG:	40 kV – 44 mA
SI:	2/3 º
RS1:	8 º
RS2:	20 mm
Soller S.:	5 º
Mono:	Kβ filter
Axis:	θ / 2θ scan
Range:	5.0 – 60.0 º
Step:	0.02 º
Speed:	20, 10, 2.4 º / min

2.4º / min = 0.5 sec/point

B (cement, fly ash) / peak search

Bragg-Brentano focusing – HyPix3000 1D

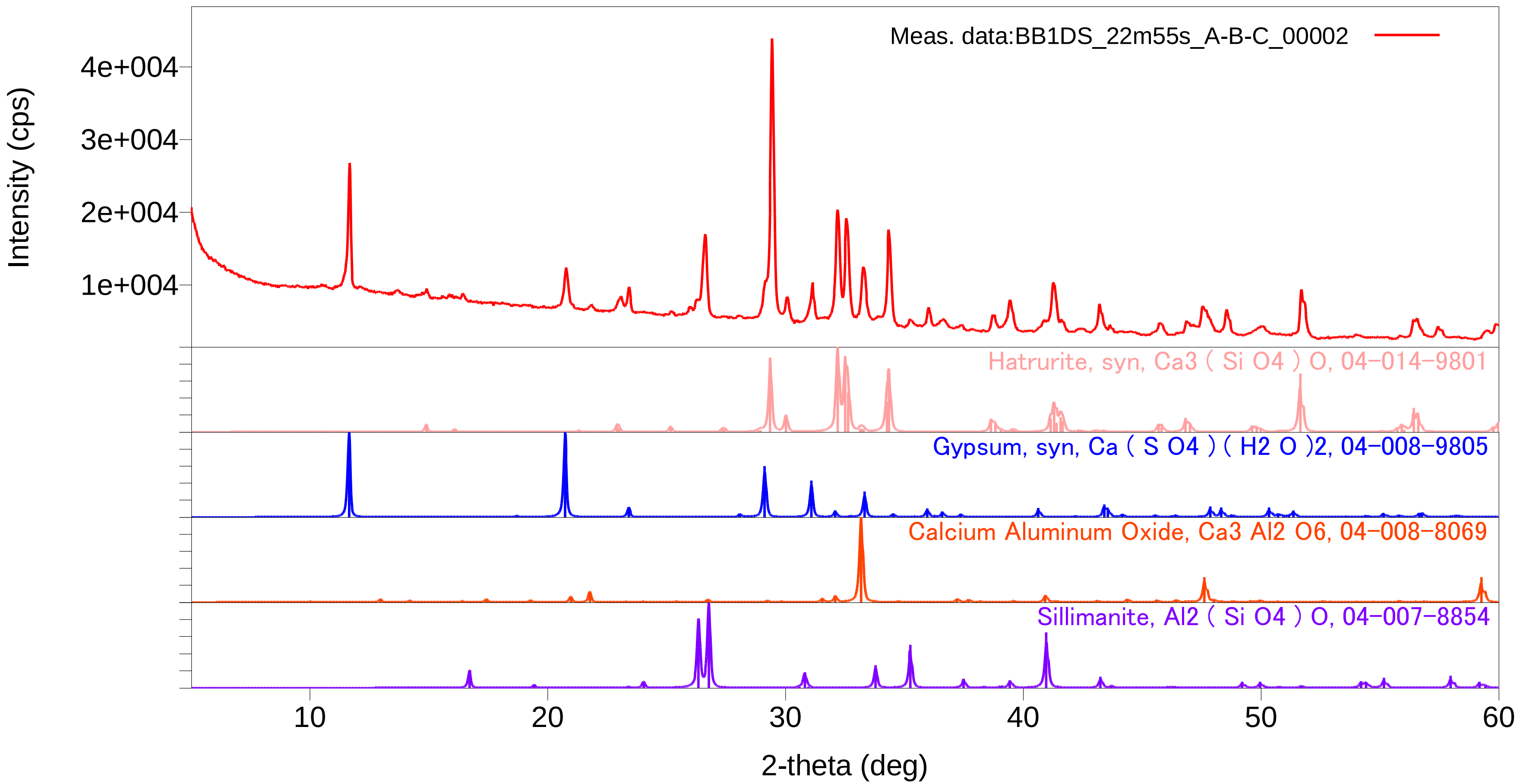


	2-theta [deg]	d-value [A]	Intensity [cps]	FWHM [deg]
1	11.6532(18)	7.5878(12)	12195(157)	0.1123(19)
2	12.165(19)	7.270(11)	274(24)	0.29(6)
3	13.69(3)	6.464(16)	347(26)	0.20(3)
4	14.93(2)	5.930(9)	593(35)	0.22(2)
5	15.853(14)	5.586(5)	485(31)	0.11(5)
6	16.467(5)	5.3789(18)	613(35)	0.14(4)
7	20.759(5)	4.2755(10)	3949(89)	0.195(4)
8	21.82(3)	4.071(5)	450(30)	0.18(2)
9	23.067(10)	3.8527(17)	1401(53)	0.274(11)
10	23.421(5)	3.7952(8)	2504(71)	0.126(6)
11	25.17(2)	3.535(3)	444(30)	0.10(3)
12	25.986(19)	3.426(2)	832(41)	0.15(2)
13	26.268(14)	3.3899(17)	1398(53)	0.171(16)
14	26.619(3)	3.3461(4)	8176(128)	0.207(3)
15	27.99(3)	3.185(4)	265(23)	0.17(4)
16	29.127(10)	3.0634(10)	2886(76)	0.26(2)
17	29.4379(14)	3.03173(14)	29568(244)	0.1344(15)
18	30.060(15)	2.9704(14)	2337(69)	0.137(14)
19	31.123(7)	2.8713(6)	4426(94)	0.109(12)
20	32.182(3)	2.7792(2)	12352(158)	0.143(4)

Total 50 peaks found

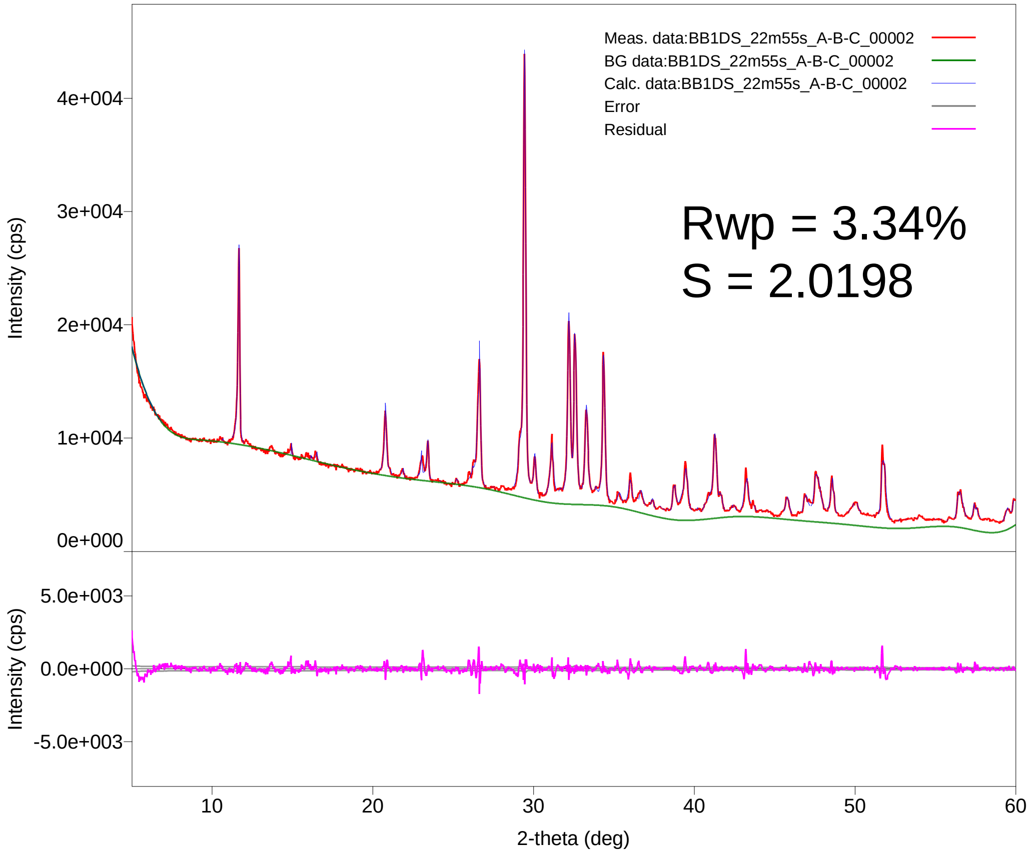
B (cement, fly ash) / phase ID

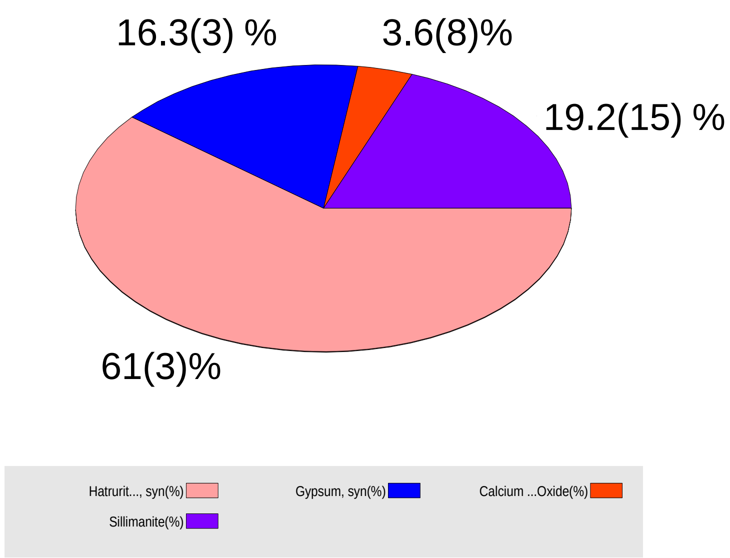
Bragg-Brentano focusing – HyPix3000 1D



B (cement, fly ash) / WPPF

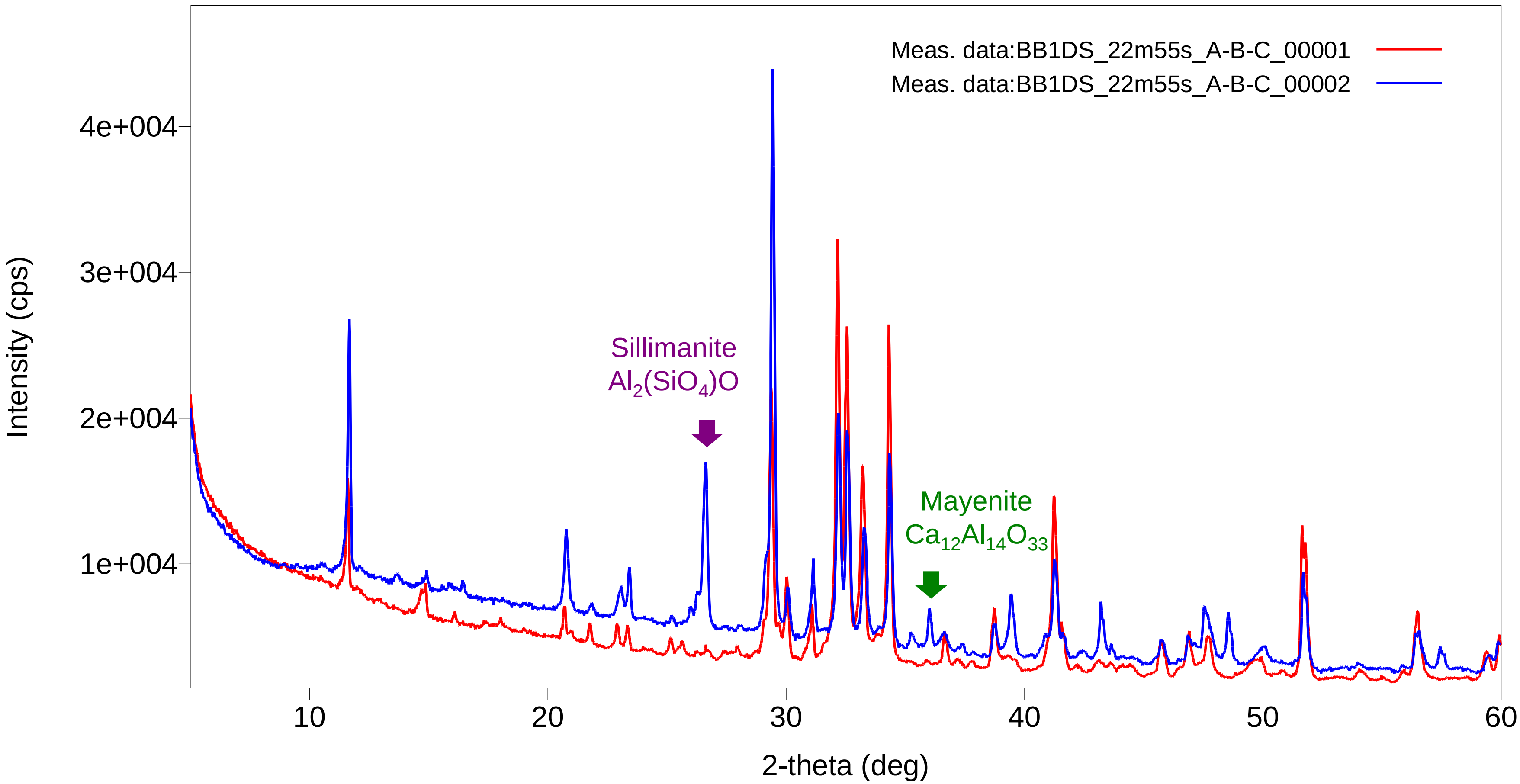
Bragg-Brentano focusing – HyPix3000 1D





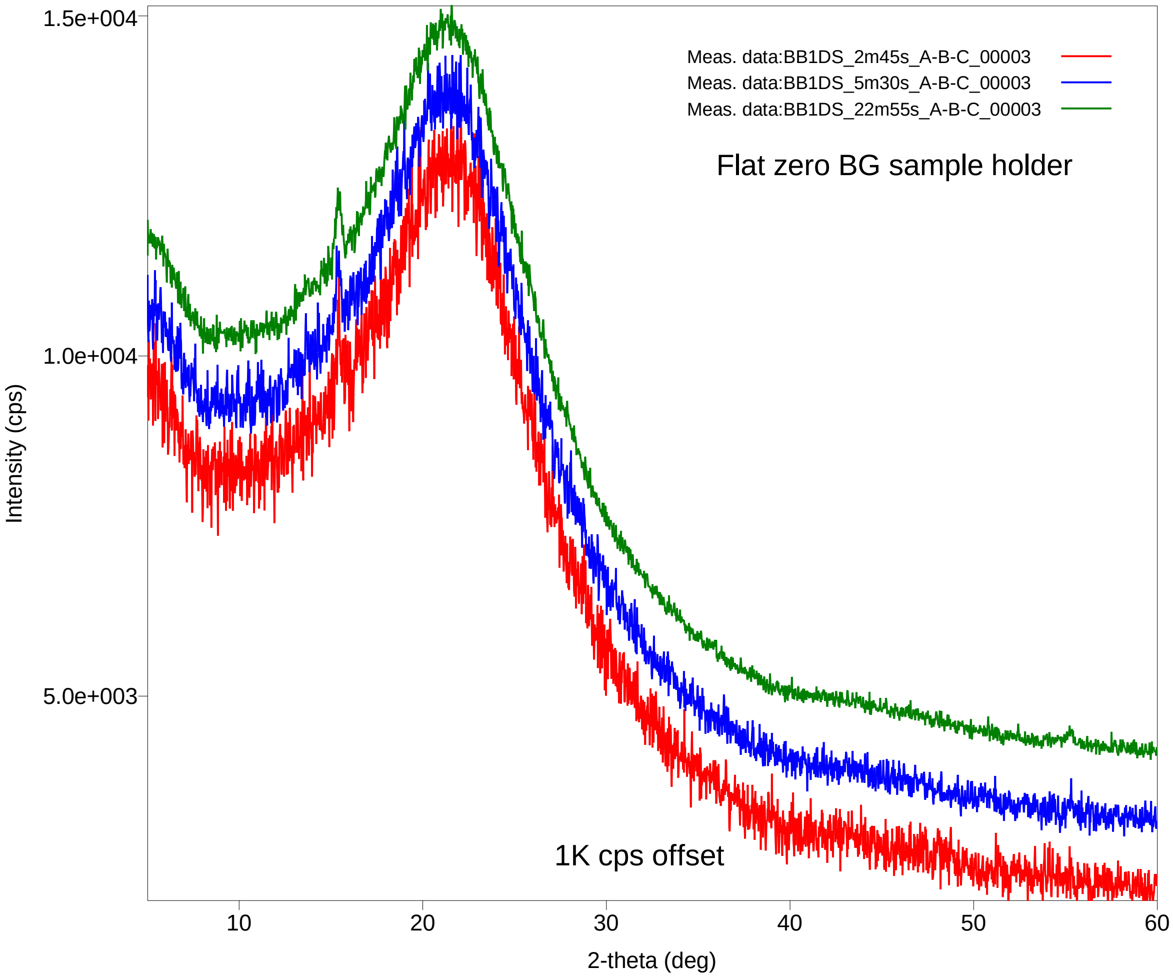
Samples A and B comparison

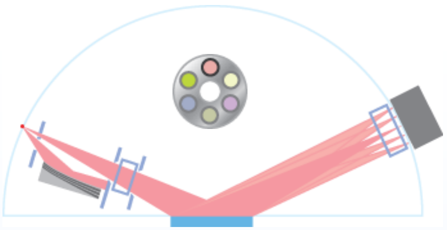
Bragg-Brentano focusing – HyPix3000 1D



C (fumed silica) / raw data

Bragg-Brentano focusing – HyPix3000 1D





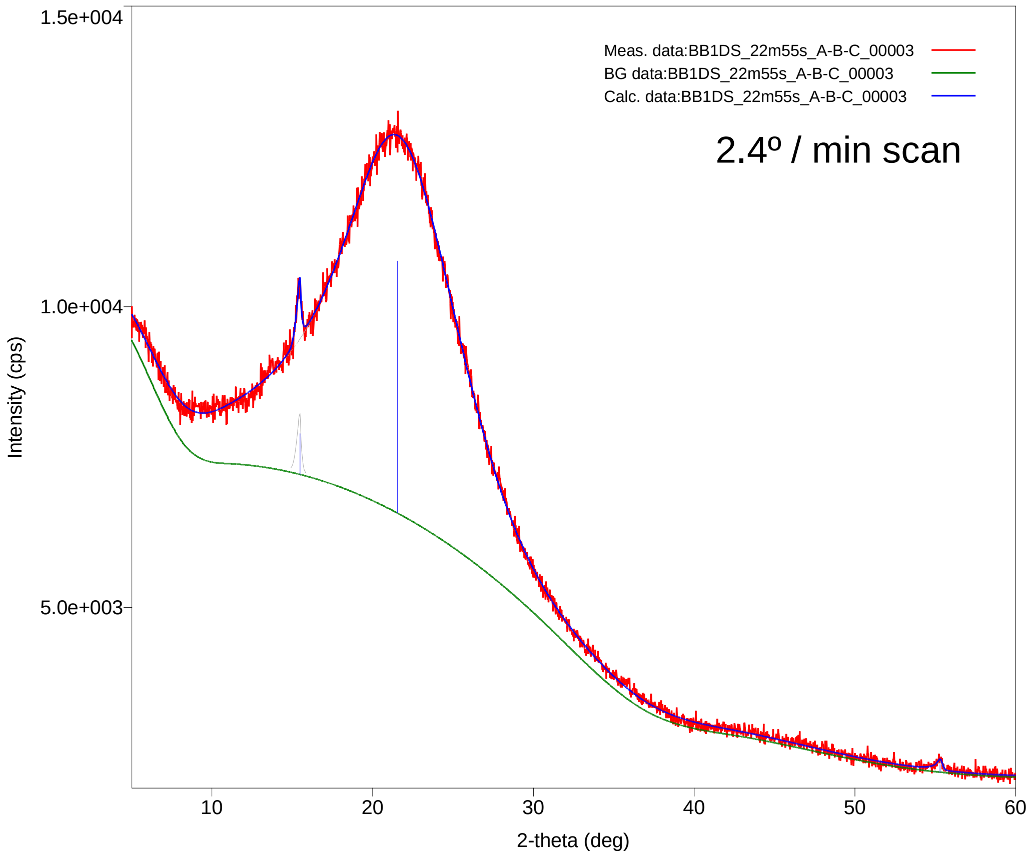
SmartLab / Standard Bragg-Brentano

Att.:	ASC-6
Spin:	5 rpm
Detector:	HyPix3000 1D
XG:	40 kV – 44 mA
SI:	2/3 º
RS1:	8 º
RS2:	20 mm
Soller S.:	5 º
Mono:	Kβ filter
Axis:	*θ* / 2*θ* scan
Range:	5.0 – 60.0 º
Step:	0.02 º
Speed:	20, 10, 2.4 º / min

2.4º / min = 0.5 sec/point

C (fumed silica) / peak search, %crystallinity

Bragg-Brentano focusing – HyPix3000 1D



	2-theta [deg]	d-value [A]	Intensity [cps]	FWHM [deg]
1	15.481(8)	5.719(3)	683(37)	0.30(3)
2*	**21.54(6)**	**4.123(11)**	**4195(92)**	**8.9(5)**
3	55.31(8)	1.660(2)	135(16)	0.40(16)

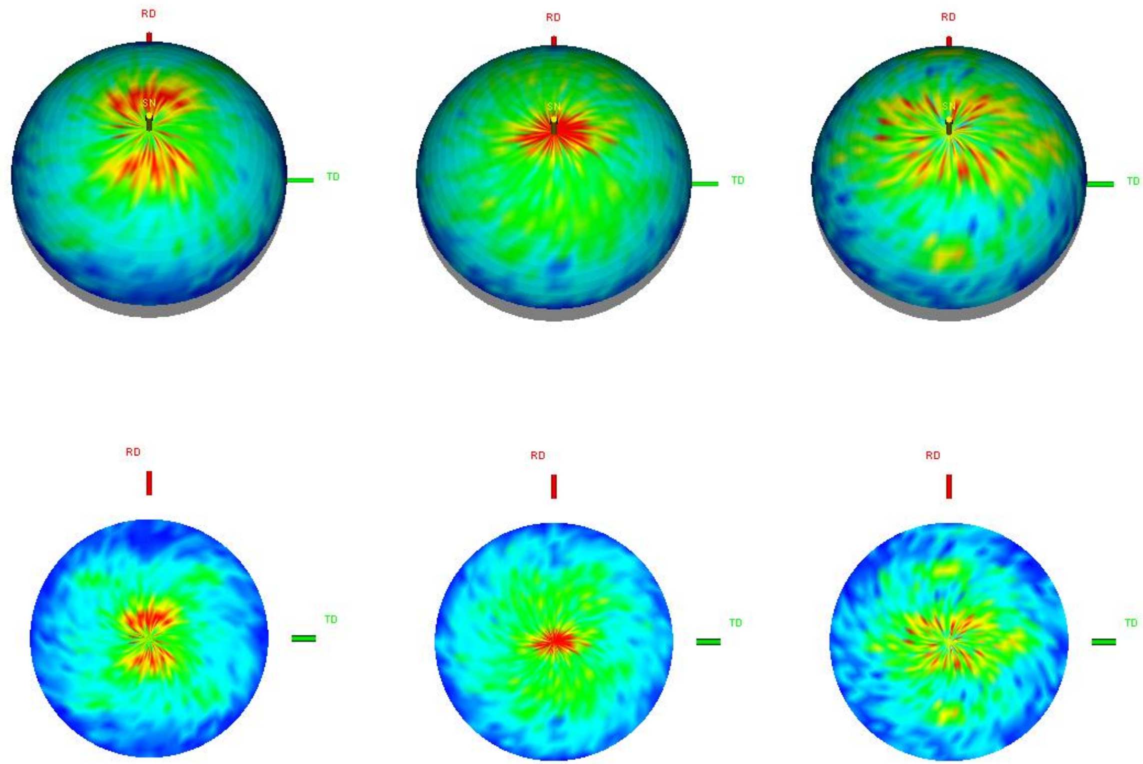
Peak # 2: amorphous peak

%Crystallinity = 0.7(2) %

Cu foil / Cu pole figures

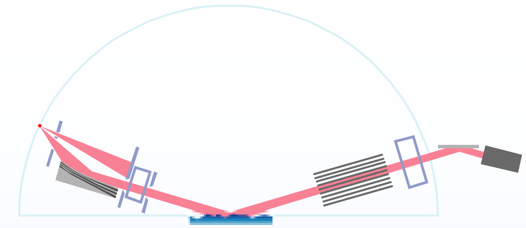
Parallel beam – HyPix3000 0D

Cu(111) @ 43.27 º | Cu(200) @ 50.35º | Cu(220) @ 74.21 º



Max. cout ~ 30K counts | Max. cout ~ 30K counts | Max. cout ~ 10K counts

Square root intensity scale

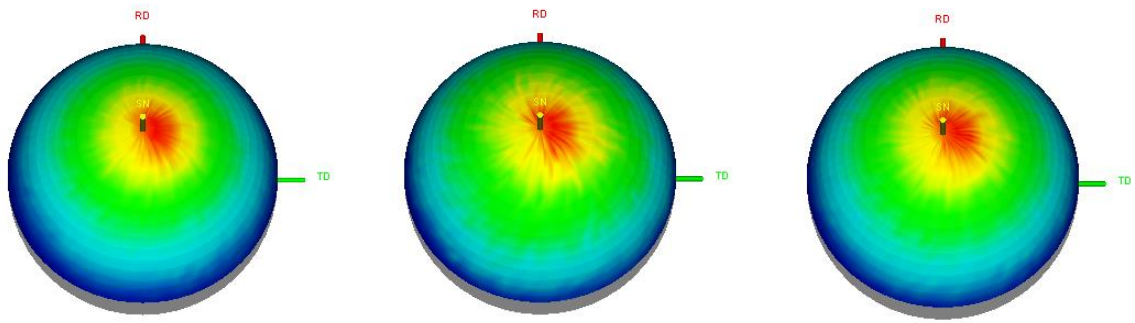


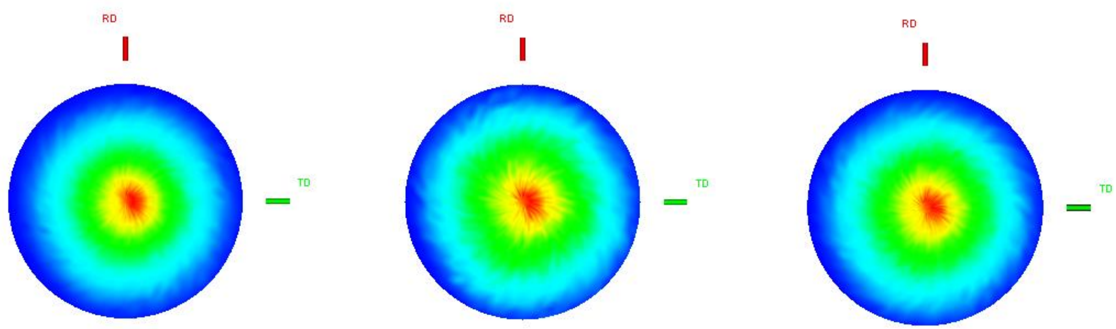
SmartLab / Standard	
Parallel beam	
Att.:	χ-φ attachment
Detector:	HyPix3000 0D
XG:	40 kV – 44 mA
SI:	1 x 2 mm
Soller S.:	5 º
RS1, RS2:	2 mm
Mono:	Graphite
α:	15 – 90 º, 5 º step
β:	0 – 390 º, 5 º step
β speed:	120 º / min
Duration:	~ 1h / reflection

Co foil / Co pole figures

Parallel beam – HyPix3000 0D

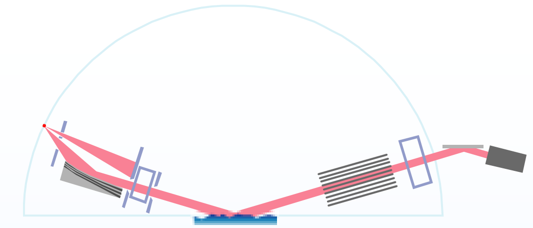
Co(100) @ 41.59 º | Co(002) @ 44.30º | Co(101) @ 47.29 º





Max. cout ~ 3K counts | Max. cout ~ 1K counts | Max. cout ~ 1.5K counts

Square root intensity scale

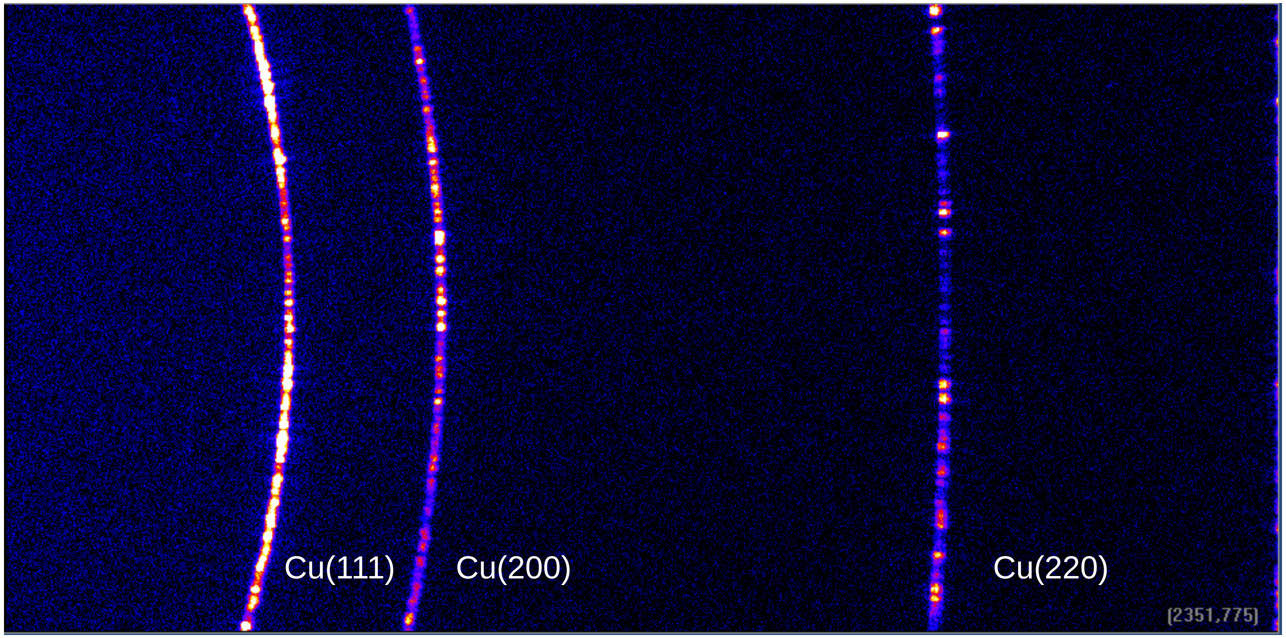


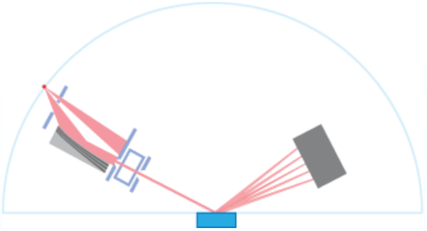
SmartLab / Standard
Parallel beam

Att.:	χ-φ attachment
Detector:	HyPix3000 0D
XG:	40 kV – 44 mA
SI:	1 x 2 mm
Soller S.:	5 º
RS1, RS2:	2 mm
Mono:	Graphite
α:	15 – 90 º, 5 º step
β:	0 – 390 º, 5 º step
β speed:	30 º / min
Duration:	~ 3h / reflection

Cu foil / 2D image

PB + CBO-*f* – HyPix3000 2D-TDI



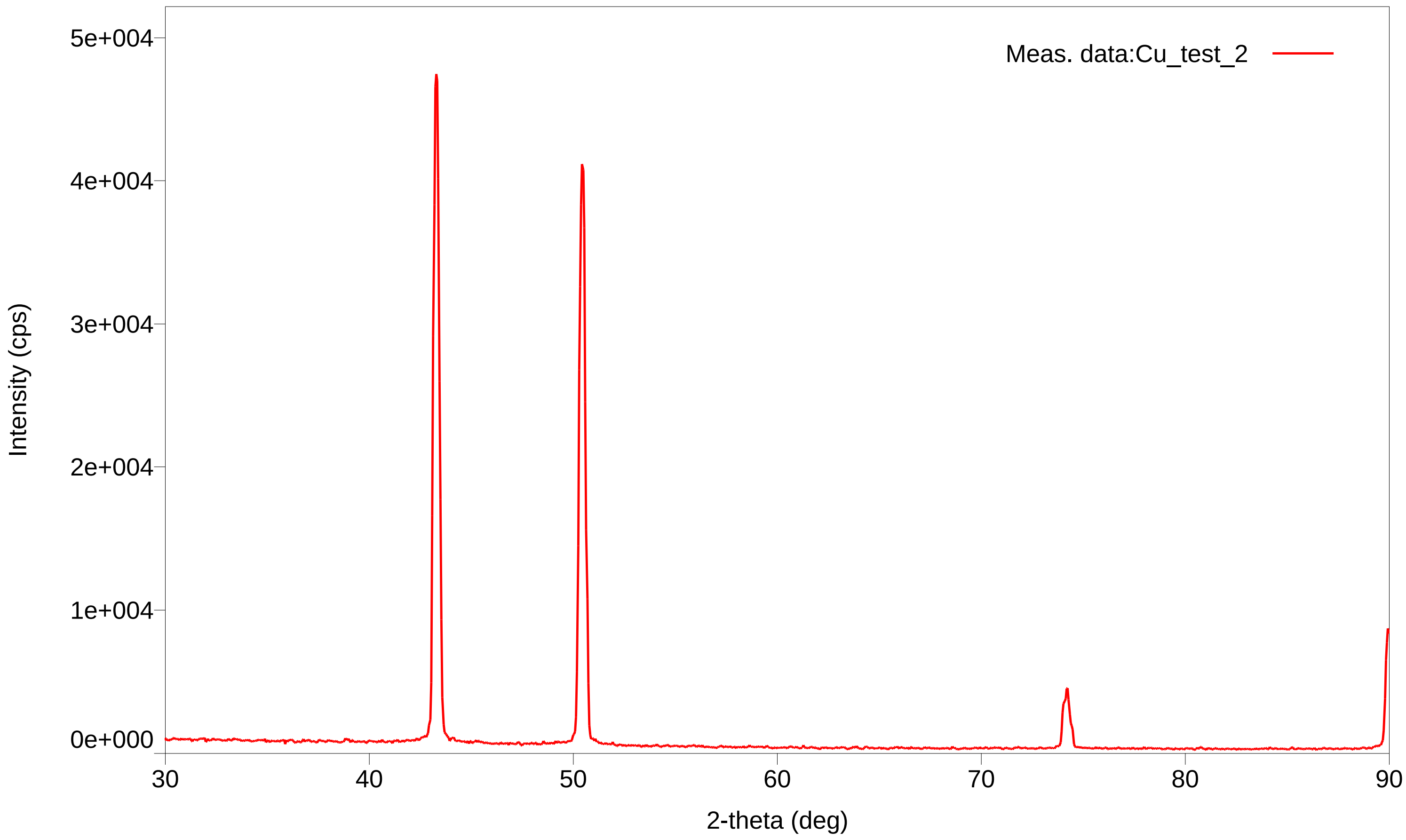


SmartLab / Standard
PB + CBO-f

Att.:	χ-φ attachment
Detector:	HyPix3000 2D
XG:	40 kV – 44 mA
SI:	1 x 0.5 mm
Camera L.:	150 mm
Axis:	θ / 2θ scan
Direction:	χ, φ = 0 º
Range:	30.0 – 90.0 º
Step:	0.05 º
Speed:	20.0 º / min

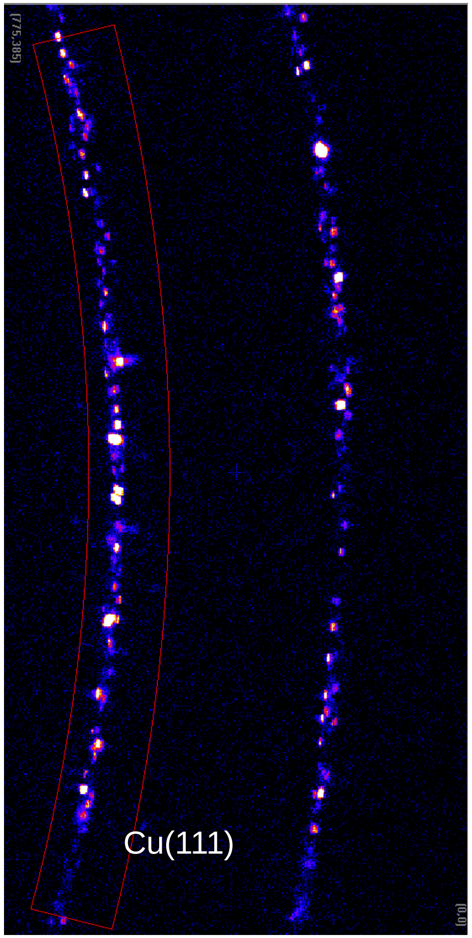
Cu foil / integrated data

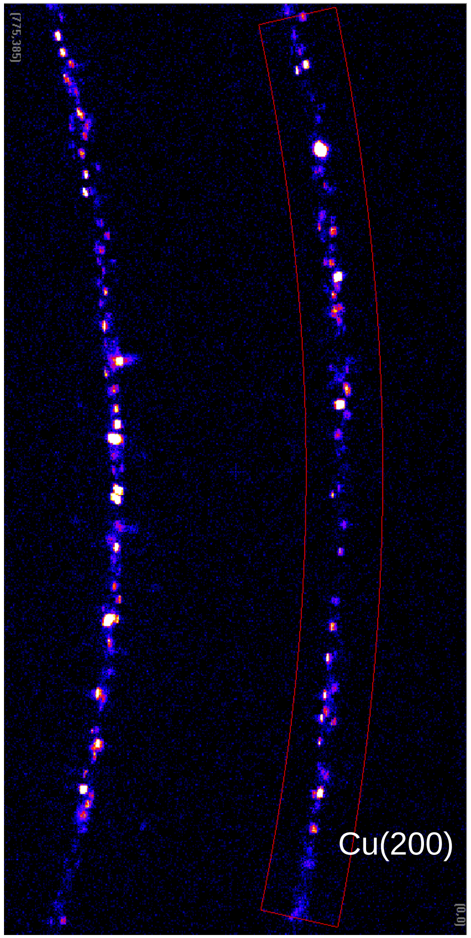
PB + CBO-*f* – HyPix3000 2D-TDI



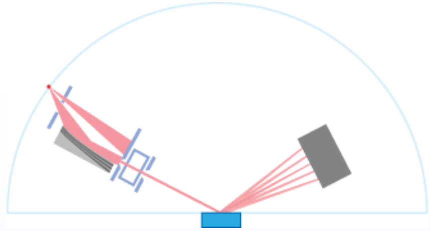
Cu foil / 2D pole figure image

PB + CBO-*f* – HyPix3000 2D





χ = 15º, φ = 0 º

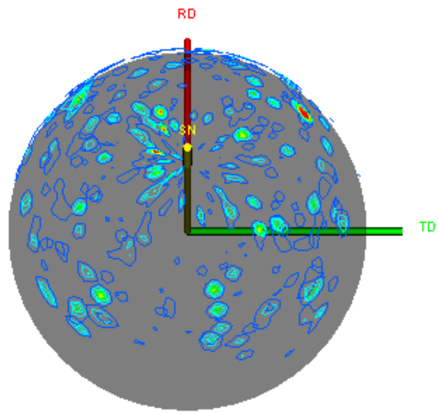


SmartLab / Standard
PB + CBO-f

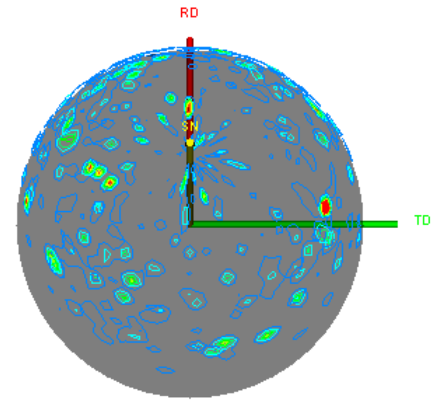
Att.:	χ-φ attachment
Detector:	HyPix3000 2D
XG:	40 kV – 44 mA
Sl:	1 x 0.5 mm
Camera L.:	150 mm
Axis:	φ scan
Range:	0.0 – 360.0 º
Step:	5 º
Direction:	χ = 15, 45, 60 º
Exposure:	10 sec
Duration:	~ 1h / 2 refs.

Cu foil / Cu 2D pole figures

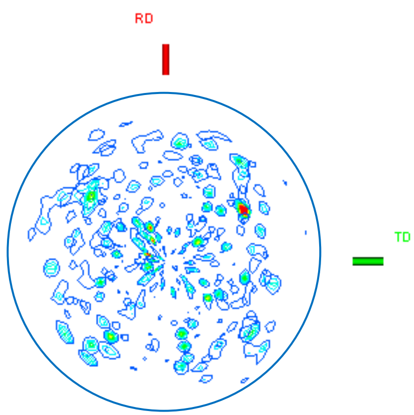
PB + CBO-*f* – HyPix3000 2D

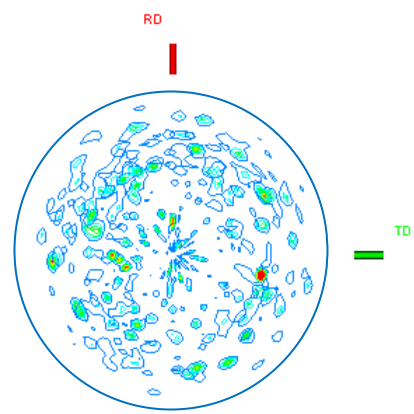


Cu(111)



Cu(200)





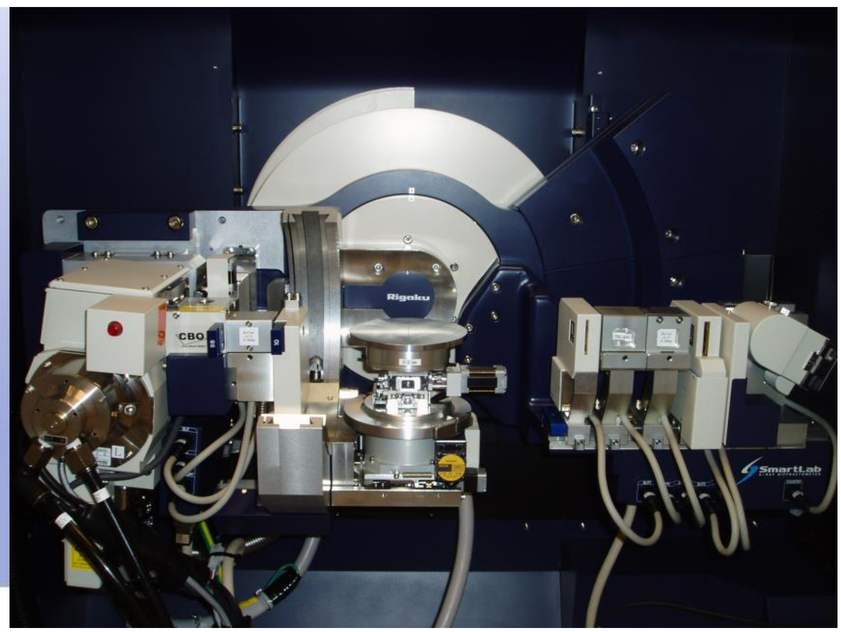
Appendix 3
Final Quotation from Rigaku

QUOTATION
XD28008

Issued To:	**Dr. Mark Holtz** **MSEC University Chair** **Professor** **Texas State University** **Department of Physics** **601 University Drive** **San Marcos, TX 78666**
Phone:	**512-245-2131**
Facsimile:	
Email:	**Mark.holtz@txstate.edu**

Date:	**July 20, 2015**
Validity:	**September 20, 2015**
Delivery:	**120 - 150 days ARO**
Shipment:	**FOB Destination to Customer's Loading Dock** – *Title and risk of loss passes to Buyer at FOB point.*
Installation:	**Included**
Warranty:	**One Year Parts and Labor**
Payment Terms:	**50% on Order, 30% on Shipping, & 20% on Installation – Net 30 Days (Pending credit approval)**

SmartLab Exterior View



SmartLab with Rotating Anode Source and Cross Beam Optics (CBO)

Commercial Summary

Section 1: SmartLab High-resolution θ/θ XRD System ....$ **531,399**
System Discount ....$ **-134,399**
Total Purchase Price Section 1 ....$ **397,000**

Notes for Purchasing Manager:

Taxes (for: Arizona, California, Colorado, Connecticut, Florida, Georgia, Hawaii, Illinois, Indiana, Maryland, Massachusetts, Michigan, New Jersey, New York, North Carolina, Pennsylvania, South Dakota, Tennessee, Texas, Utah, Virginia, Washington, Wisconsin) will be added to invoice if applicable. If Buyer claims tax exempt status, Buyer agrees to provide Rigaku Americas Corporation (Seller) with a tax exemption certificate acceptable to local taxing authorities in the jurisdiction concerned.

Seller offers to sell to Buyer, and Buyer agrees to purchase from Seller, the goods and services described below, subject to the terms and conditions stated on the face of this Quotation and Seller's standard terms and conditions, attached. Seller hereby objects to any additional or different terms stated in Buyer's request for quotation, purchase order, or any other document of Buyer. Any modification of these terms of sale must be specifically agreed to in writing by Seller. This contract is binding upon Seller's receipt of Buyer's Purchase Order for same. Please address Purchase Order to Rigaku Americas Corporation to the address at the bottom of this page or e-mail to purchaseorder@rigaku.com .

Prices are listed in U.S.A. dollars.
Prices are based on quoted payment terms.
Prices and specifications subject to change without notice.

Inside delivery is not included. If inside delivery is required, an additional charge will apply. When accepting delivery, please note on transport documents any shortage or damage, and advise Rigaku Americas Corporation immediately at: support@Rigaku.com .

Michael A. Holcomb

Mike Holcomb
Southwest Regional Account Manager
Rigaku Americas Corporation
281-610-3558
Michael.Holcomb@Rigaku.com

<table>
<tr><th>ITEM</th><th>QTY</th><th>PART NUMBER</th><th>DESCRIPTION</th><th>PRICE</th></tr>
<tr><td colspan="3">Section 1</td><td colspan="2">SmartLab X-ray Thin Film Diffraction System</td></tr>
<tr><td>1</td><td>1</td><td>2080B201</td><td>X-ray Generator System
The SmartLab X-ray Diffraction System includes a highly stable and reliable sealed tube x-ray generator that is fully integrated within the automated diffraction system and is compatible with the full range of SmartLab goniometer configurations.
Specifications
• 3.0 kW Continuously Rated Output Power
• Computer-Controlled and Manual Operation
• Voltage: 20-60 kV, 2 kV step
• Current: 2-60 mA, 2 mA step
• Stability: ± 0.005 % for 10 % input power variation
• Integrated table top, enclosure support stand, and system electronics rack
Dimensions
• Including tool stand 47” W x 50” D x 73” H
Safety Features
• Cooling Water Flow and Pressure Detection
• Generator Overload Detection
• Tube Voltage Detection
• Emergency Stop Switch
• Leak Current Breaker</td><td>Included</td></tr>
<tr><td>2</td><td>1</td><td>4620A101</td><td>Radiation Enclosure
• Steel construction with integrated lead panel direct beam stop.
• Safety interlocked with electromagnetic shutter mechanism.
• Sliding front access doors with high/low leaded-acrylic windows.
• Lighted interior.</td><td>Included</td></tr>
<tr><td>3</td><td>1</td><td>R01-29-0202</td><td>Cu X-ray Tube
Tube shield is supplied with (1) Electromagnetic Shutter. Tube comes with extra o-ring seals.
Specifications
• 2.2kW, Long-Fine Focus, X-ray Tube
• Focal Spot 0.4 mm x 12.0 mm</td><td>Included</td></tr>
<tr><td>4</td><td>1</td><td>CHILLER-PENDING</td><td>Heat Exchanger (Air Cooled or Water Cooled)
Water chiller system for cooling of the X-Ray source.</td><td>Included</td></tr>
</table>

ITEM	QTY	PART NUMBER	DESCRIPTION	PRICE
5	1	**Included with 2080B201**	**Incident Beam Optics** **Cross Beam Optics (CBO) Technology** User selectable parallel beam and focusing optical configurations for asymmetric and symmetric scanning geometries. Permanently mounted, permanently aligned parabolic multilayer x-ray mirror is compatible with all optical and goniometer configurations. **Specifications** **High-resolution Parallel Beam Optics** • Laterally graded incident beam multilayer x-ray mirror. • Automated mirror control and alignment. • CBO Selection Slit: Parallel Beam • Variable Incident Slit: 0.05 – 7.0 mm, 0.01 mm step • Height Limiting Slit: 2.0, 5.0, 10.0, and 15 mm **Bragg-Brentano Para-Focusing Optics** • CBO Selection Slit: Bragg-Brentano • Variable Divergence Slit: 0.05 – 7.0 mm, 0.01 mm step • Height Limiting Slit: 2.0, 5.0, 10.0 mm • Soller Slits: 5° axial divergence	**Included**
6	1	**2680B111**	**Ge (220) 2-Bounce Incident Beam Monochromator** Ge (220) 2-bounce high-resolution channel-cut incident beam monochromator for high-resolution parallel beam measurements of the crystal structure of imperfect materials. Fully automated channel cut Ge crystal provides precise alignment and user-friendly operation. **Specifications** • Monochromator: Ge (220) 2-bounce channel-cut crystal • Incident beam divergence: 32 arc sec	**Included**
7	1	**2431D201** **2431C303** **C387-0076**	**2D Optics** **Collimator Holder** **PB 0.3mm Selection Slit** **0.2 mm Collimator**	**Included**

ITEM	QTY	PART NUMBER	DESCRIPTION	PRICE
8	1	**Included with 2080B201**	**Goniometer System** **SmartLab High-Resolution Vertical θ/θ 4-Circle Goniometer** High-resolution vertical theta-theta goniometer system with open architecture design for horizontal sample mounting and measurement. Supports the full range of multipurpose sample stages, accessories, and optical configurations. Engineered for highest resolution measurements including triple-axis measurements on highly perfect epitaxial materials. Supports sealed tube or rotating anode x-ray sources. **Specifications** • High-precision, vertical θ/θ geometry (horizontal sample mounting) • Optical encoder controlled • Fully automated alignment • Independently controlled θ_s (source) and θ_d (detector) axes • Measuring range: -3 – 160° (2θ) • Scanning speed: 0.01°/min - 20°/min (θ_s, θ_d) • Slewing speed: max. 250°/min (θ_s, θ_d) • Step Resolution: 0.0001°(θ_s, θ_d) • Scanning Method: θ_s / θ_d independent or coupled • Accessories Kit with: ⇒ Standard Sample Holder Attachment ♦ Stage for the powder and bulk sample holders. ♦ Includes electronics for the attachment-type sensor. ⇒ Sample Holder for 4" wafer ♦ Flat-surface wafer sample holder for up to 4" inch wafer ⇒ Sample-Stage Spacer for 0-3mm thick sample ♦ Can be placed between the sample holder and the attachment to adjust the Holder height according to the sample thickness. ⇒ Center Slit for alignment ⇒ Si Reference Standard ⇒ Hex screwdriver for optics units mounting	**Included**

ITEM	QTY	PART NUMBER	DESCRIPTION	PRICE
9	1	**Included with 2080B201**	**Sample Stages** **SmartLab Horizontal Sample Stage and Eulerian Cradle** Samples are easily mounted on the horizontal sample stage without the need for clamping or vacuum chucking. Sample remains perfectly flat and stationary throughout the measurement, which keeps the sample from bending, bowing, or vibrating during analysis. High precision Z-axis is combined with the open Eulerian cradle, which provides χ and ϕ axes with a large coverage of reciprocal space. **Specifications** • High-precision motor driven sample stage • Fully automated sample alignment • Z: -4 ~ 1 mm / 0.0005 mm step • χ: -5 ~ 95° / 0.001° step • ϕ: -720 ~ 720° / 0.001° step	**Included**
10	2	**SH-SI-RECTA**	**Low Background Sample Holder for Basic Sample Stage, Rectangle, No indent**	**Included**
11	1	**2680A212**	**100mm XY Sample Stage** XY stage mounts directly on the SmartLab high precision Z-stage with no alignment. XY mapping is possible over entire 100mm sample surface size. **Specifications** • X,Y: ± 50 mm / 0.0005 mm step • Sample Size: 200 mmϕ (8" ϕ) diameter maximum • XY Mapping: 100 mmϕ (4" ϕ) diameter area	**Included**
12	1	**2680J111**	**Small Angle X-ray Scattering (SAXS) Attachment** Unique SAXS optical system using CBO optics technology allowing the user the ability to switch from Bragg-Brentano to Parallel Beam SAXS optics in seconds without removing the x-ray mirror and without any realignment. Transmission and reflection sample stages and optical configuration allow measurements to be performed on length scales as long as 100nm on a conventional wide angle x-ray diffractometer system. Applications include pore and particle size distribution analysis, measurement of long periodicities, and nanoparticle modeling. Patented by Rigaku. **Specifications** • CBO Selection Slit: SAXS Selection Slit • Resolution: 1 ~ 100 nm with Cu Kα radiation • Vacuum Path: Sealed, scattered beam • Stage: Sample Stage for transmission geometry; reflection SAXS done with included high-precision Z-stage.	**Included**
	1	**2680F201**	**Receiving Slit for SAXS – 20 mm x 8 mm**	
	1	**2680F202**	**Receiving Slit for SAXS – 20 mm x 10 mm**	
	1	**2680F203**	**Receiving Slit for SAXS – 20 mm x 15 mm**	

ITEM	QTY	PART NUMBER	DESCRIPTION	PRICE
13	**1**	**XRD-AP-DHS1100**	**Anton Paar DHS 1100 Domed Hot Stage for SmartLab** The DHS 1100 is an advanced heating stage for use with SmartLab with Eulerian Cradle or In-plane Diffraction goniometers. The DHS 1100 can be used for temperature-induced phase transition investigations, texture measurements, and stress analysis at elevated temperatures. The unique dome-shaped X-ray window made of graphite allows you to analyze samples under vacuum and under inert gas to avoid oxidation or other chemical reactions of the sample at high temperatures. **Specifications** • Operating temperature: 25 °C to 1100 °C • Temperature measurement: Pt-10% Rh-Pt thermocouple • Atmospheres: Vacuum (10 -1 mbar), air, inert gas, nitrogen • Max. operating pressure: max. 0.3 bar above atmospheric pressure • Possible scattering angle: 0 to 166° 2Θ, 0 to 85° Psi,0 to 360° Phi • Sample holder material: Aluminum nitride • Sample diameter: Maximum 25 mm • Dome Material: Graphite • Measurement geometry: Reflection **Includes** • DHS 1100 domed hot stage • Set of Powder Sample Carriers for DHS 1100 • TCU 200 temperature control unit • Air service unit • Subkit with vacuum pump	**Included**
			Diffracted Beam Optics	
14	**1**	**Included with 2080B201**	**Diffracted Beam Optics Assembly** Modular beam path suitable for a wide range of diffracted beam optical configurations including parallel slit analyzers and Ge analyzer crystals, and dual receiving slits. **Specifications** • Receiving Slit 1: Computer-Controlled, 0.05 mm - 20 mm, 0.01 mm step • Parallel Slit Analyzer: 0.5° Angular Divergence • Receiving Slit 2: Computer-Controlled, 0.05 mm - 20 mm, 0.01 mm step • K_β Filter: Nickel for Cu Radiation • Attenuator: Computer-Controlled, Four attenuators w/ different absorption rate	**Included**
15	**1**	**2680C111**	**Ge(220) x 2 analyzer, diffracted beam** For triple-axis measurements when combined with optional Ge(220) x 2, Ge(220) x 4, or Ge(440) x 4 monochromators.	**Included**

ITEM	QTY	PART NUMBER	DESCRIPTION	PRICE
16	1	**Included with 2080B201**	**Detectors** **Scintillation Detector** A high-efficiency scintillation counter and measuring electronics provide high-count rate linearity. Pulse-height analyzer (PHA) and detector high-voltage settings are computer controlled. **Specifications** • Linearity: 700,000 cps or better • Electronics: Pulse Height Analyzer, Computer-Controlled • Detector High Voltage, Computer-Controlled • Dead time correction: Computer-Controlled and Automated	**Included**
17	1	**A00001644**	**HyPix-3000 Hybrid Pixel Array 0D/1D/2D Detector** The HyPix-3000 hybrid pixel array detector is the most ideal detector for x-ray diffraction available today. The HyPix-3000 combines a large active area with a small pixel size, ultra high dynamic range and global count rate with direct photon counting sensitivity, virtually no noise, high detector efficiency, superfast readout, and high energy resolution in a single detector. Seamless switching from 2D scanning mode to 2D snap shot mode to 1D scanning to 1D snap shot to 0D mode is fast and easy with a single detector allowing the user to utmost experimental flexibility for a truly multipurpose XRD system for the widest range of applications. Featuring dual energy discriminators, the user can adjust the energy threshold to suppress fluorescence and to eliminate cosmic rays and white radiation for optimized signal-to-noise. The HyPix-3000 is manufactured directly by Rigaku and beautifully integrated into the SmartLab. **Specifications** • Hybrid pixel array multi-dimensional 0D/1D/2D detector • 2984mm2 active area • $2.9x10^{11}$ cps global count rate / $1x10^{6}$ cps local count rate • 100µm x 100µm pixel size • 298,375 total pixels • 32 counter bit • 2 channel threshold • 3.2msec and “zero dead time” 17nsec readout speeds • 99% efficiency for Cu radiation • 20% energy resolution • 147mm (W) x 93mm (H) x 180mm (D) dimensions • 2kg weight **Includes** • HyPix-3000 • Server PC & Software • Frame Grabber, LAN Board, and Link Cable • Incident Soller Slit Open (2680D115) • Beam shaping slits (2680G111 • Horizontal mount for HyPix-3000 • Alumina powder ***Requires: 2DP Data Processing Software***	**Included**

ITEM	QTY	PART NUMBER	DESCRIPTION	PRICE
18	1	**PC-SL PC-PRINTER PC-MONITOR-19”**	**Computer, Monitor and Printer** PC Computer for instrument control and data processing. **Specifications** • Intel Core™ i7 Processor (3.4 GHz) • 4.0 GB SDRAM • Video, 256MB ATI RADEON HD3450 • Internal Audio Speaker • 19” ultra sharp Flat Panel LCD • Dual Monitor Capability • 500 GB hard drive with 16MB DataBurst Cache • 16X DVD+/-RW, will read/write CD’s • 8 USB Ports, 6 on back, 2 on front • Keyboard, USB 2 Button Scroll Mouse and Pad • **Microsoft Windows 7 PRO, 32 bit** ***(64 bit will not work)*** • Microsoft Office 2013 Basic • Adobe Acrobat Standard • Color Printer with Cable • Up to 4 Serial Ports needed depending on configuration • **Two (2) Ethernet Ports required** • 3 yr Basic Limited Warranty, 3 yr NBD On-Site Service from Dell ***Notes: Above configuration to be provided. Customer to ensure networking capabilities provided to facilitate installation. Includes software integration and testing***	**Included**
19	10	**Included with 2080B201**	**SmartLab Studio Software for SmartLab** SmartLab Studio is a one click central command software solution that fully automates data collection, data processing, data analysis, and reporting of results. SmartLab Studio seamlessly integrates the SmartLab optical recognition technology and SmartLab Guidance 2.0 instrument control and data collection software with all Rigaku data analysis software programs resulting in unmatched automation and ease of use. Using Data Browser, Application Launcher, and Recipe Editor features within SmartLab Studio, the user is guaranteed to obtain high quality results quickly and easily in only one click which saves valuable time and resources, reduces errors, and increases productivity. Patent Pending. **Data Browser** • Data files shown in thumbnail images or detailed information displays . • Available data analysis programs are highlighted for selected data files. • File headers include measurement and analysis conditions. • Find data based on data type, date, owner, etc. • Show history of data collection and analysis. **Application Launcher** • No more redundant login screens with automatic login. • Launches proper data analysis software for selected data file automatically. • Automatic conversion of 2D data and launched as 1D data for analysis in PDXL.	**Included**

ITEM	QTY	PART NUMBER	DESCRIPTION	PRICE
		Included with 2080B201 Continued	**Recipe Editor** • User can customize fully automatic data collection, data processing, data analysis, and reporting of results. • Batch processing of multiple data sets simultaneously.	
20	**1**	**Included with 2080B201**	**SmartLab Guidance™ 2.0** SmartLab Guidance 2.0 software was created by capturing the actual work flow of all the steps of an expert application scientist for a particular application. These steps were then coded into Guidance so the user receives the benefit of this embedded experience and intelligence which is built into Guidance. Through the SmartLab hardware optical recognition technology, Guidance knows how the instrument is configured enabling it to recommend the best optical configuration and measuring conditions for the specific sample type and desired result. The user is guided through set up by SmartMessages™. Sample and system alignment are automatic. Guidance improves ease of use and productivity to get more and better results. Patented by Rigaku. **Configuration** • Fully automatic system alignment • Goniometer and detector settings • Attachment configuration definitions • Optics definitions **Manual Measurement** • Enables user control the goniometer and attachment axes as well as setting of the detector high voltage. • Used to check system alignment. • May be used to perform simple measurements. **Standard Measurement** • Allows up to fifty different sets of measurement conditions to be defined by the user. These conditions are stored for later use and can be edited. • Multiple measurement conditions can be applied to the sample and up to six samples can be measured when using the optional sample changer. • Real-time data display is provided along with the ability to suspend or abort running measurements. **Included** • SmartLab Studio recipe compatibility. • Application wizard. • Optical recognition of instrument configuration in real time with virtual goniometer display. • SmartMessages to guide user to add or remove optical components, sample stages, and accessories. • Conflict detection with specific component identification to ensure optimal hardware set up every time. • Control of (optional) programmable temperature controller for user-programmed heating and cooling profiles.	**Included**

ITEM	QTY	PART NUMBER	DESCRIPTION	PRICE
21	10	9240J765 9240J704 9240R851 9240R804	**PDXL Comprehensive Analysis Package** **Includes: PDXL Basic Analysis Package** **Display Features** • Zoom, reset, and pan. • Multiple pattern overlays in 2D and 3D. • Hiding analysis results to show raw data only. • Switching 2 theta axis to S or Q. • Customizing line colors, widths, and markers. • Windows clipboard support for copy and pasting into other applications. • Thumbnail viewing. • Drag and drop from Explorer. • Access to your ICDD database for overlays and card printing. • View crystal structures in 3D with real-time manipulation. **Data Reduction Features** • Automatic data reduction and peak list reporting. • Sonneveld-Visser and polynomial function background elimination. • Rachinger method Kα2 elimination. • Automatic and/or manual peak finding. • Peak-top and second-derivative peak finding. • Gaussian moving average, Savitzky-Golay, optimized Gaussian moving average, and B-spline smoothing. • Beam footprint and absorption corrections for variable slit. • Absorption correction for capillary. • LP correction for monochromators. **Data Analysis Features** • Simultaneous processing of multiple patterns. • Automatic individual parameter fitting. • RIR quantitative analysis using imported phase information. • Crystallite size determination using a single diffraction peak (Scherrer's equation) with and without an external standard reference material. • Boolean search of ICDD PDF databases. **Data Input/Output Features** • Universal ASCII pattern file import and export. • Detailed processing logs. • Import/export d-I and IUCr CIF files. • Microsoft Word report file creation. • Online PDF manual. • Easy creation and management of searchable database from ICDD and user defined phases • d-I list editing and file import.	**Included**

ITEM	QTY	PART NUMBER	DESCRIPTION	PRICE
		9240J765 9240J704 9240R851 9240R804 Continued	**Advanced features module includes additional crystallographic capabilities for a wide range of applications.** **Crystallinity determination module** • % Crystallinity determination using whole pattern fitting. **Crystallite size and lattice strain determination module** • Instrumental broadening deconvolution using internal or external standard reference material. **Cell refinement module** • Cell refinement using internal or external standard reference material. • Standardless cell refinement using theoretical systematic error correction. • Plots of cell refinement results for multiple samples or measurement conditions. **Residual stress analysis module** • Residual stress analysis using the sin2ψ method. • Stress constant calculation based on diffraction angle, Poisson's ratio, and Young's modulus. • Residual stress analysis based on a specified stress constant.	
22	**10**	**9240J702 9240R802**	**PDXL Qualitative Analysis Package** **Search Match Features** • Interface to ICDD PDF-2. PDF-4 and COD databases. • Provisions to carry sample information such as chemistry, cell constants, density, etc. in the user file. • Powerful line and profile-based hybrid search/match algorithm, with before/after chemistry filter, control of sensitivity to lattice parameter, focus on minor phases, and consideration of preferred orientation. • GUI result display with the d-I overlay tools. • Independent GUI result display with zoom and pan support. • "Flexible cell" algorithm for solid solution and iso-typical phases. • Residual display and repeat of search/match with specified peaks. • Automatic selection of best FOM phases. • Sort and tree display on similarity for simple phase identification. **Requires PDXL Basic and Database**	**Included**

ITEM	QTY	PART NUMBER	DESCRIPTION	PRICE
23	10	9240J711 9240R911	**PDXL Whole Pattern Fitting/Rietveld - Educational** Utilizes the Rietveld method for quantitative analysis, lattice constant determination, and structure refinement using the whole XRD pattern. Physical scattering models are built using actual crystal structure parameters for the various phases. Non-linear least squares optimization procedures bring this model into agreement with your measured pattern by adjusting parameters of the model. These parameters include background, profile shapes, lattice constraints, atom coordinates, site occupancy and thermal factors. WPF nicely compliments the model building in cases where a structure may be unknown, yet a good single-phase pattern is available. **Features** • Pattern simulation and fitting using atomic coordinates. • Full physics simulation includes anomalous scattering, and atomic thermal tensors. • Use structure and/or structureless phase data. • Peak Decomposition by Pawley Method. • Automatic initial parameter determination. • Graphical displays of refinement progress and results. • Auto load of structure data from FIZ-ICSD database. • Lattice constant determination with corrections of instrumental and experimental aberrations, with/without internal phase standard. • Quantitative analysis with/without amorphous content, absorption, and preferred orientation correction. • Output including refinement results, presentation printouts and reports. • Polynomial and B-spline background models. • Bragg-Brentano focusing method, trigonometric, polynomial systematic error models. • Pseudo-Voigt and Pearson VII profile models. • March-Dollase and harmonic function models. • Intelligent constraints on atomic coordinates at special sites, occupancies, and thermal factors. • Constraint models for profile FWHM, shape, asymmetry. • Calculate bond distances and angles of near coordinated atoms. • Fourier maps calculation and display. • Difference Fourier maps calculation and display. • Maximum Entropy Method calculation and display. **Requires PDXL Basic (minimum, user database CIF's only)** **OR** **COD** **OR** **ICDD PDF-2 with ICSD-NIST (Preferred)** **OR** **ICDD PDF-4**	Included

ITEM	QTY	PART NUMBER	DESCRIPTION	PRICE
24	1	**ICDD-PDF2-EDU**	**ICDD PDF-2 Database - Educational** **Database Features** • Includes 120,000 compounds with over 95,000 inorganic phases. • The PDF-2 database is a collection of single-phase X-ray powder diffraction patterns in the form of tables of interplanar spacings (d) and relative intensities (Int) and chemical name and formula as well as mineral name, if applicable. • In addition, Miller indices, cell data and physical properties are listed, together with references for source information, where such data are available. • The PDF-2 database also contains calculated patterns obtained from the Inorganic Crystal Structure Database (ICSD). Powder patterns were calculated from atomic coordinates for almost 40,000 compounds.	**Included**
25	10	**9240H403** **9240R406**	**3D Explore RSM & PF Display and Analysis Software** Three dimensional display and data process of both Reciprocal Space Map (RSM) and Pole Figure (PF) data. **Features** **Reciprocal Space Maps** • 1D, 2D, and 3D reciprocal space map display • Raised and/or flat topography plot and cross section plot • Goniometer axes and Q axes conversion • Overlay of multiple reciprocal space maps • Simultaneous data process of multiple data sets • Advanced data process and mismatch analysis **Pole Figures** • Raised and flat topography plot and cross section plot • Reciprocal space sphere display of orientation • Rotation correction of alpha and beta • Advanced data process and pole search analysis	**Included**

ITEM	QTY	PART NUMBER	DESCRIPTION	PRICE
26	10	9240H115 9240R116	**GlobalFit Rocking Curve and Reflectivity Software SET** **GlobalFit Extended Rocking Curve Simulation** Based on the extended dynamical diffraction theory for characterization of thickness, lattice mismatch, and chemical composition in epitaxial (single-crystal) thin films. **Data display and export features** • Display of rocking curve. • Zoom and pan. • Copying of images and data profiles to Clipboard for reporting. • Layer structure display. • Exporting text data files. • Automatic HTML report creation. **Analysis features** • Simple flow bar interface. • Rocking curve analysis and optimization of concentration and thickness based on an epitaxial multilayer model. • Global fitting method to automatically optimize the initial fitting parameters. • Modeling for all space groups. • Modeling for symmetric and asymmetric reflections with and without miss-cut. • Extended rocking curve simulation algorithm for better approximation of grazing incidence reflections than conventional two-wave approximation algorithm. • Modeling for gradual or random change of concentration and period of superlattice. **GlobalFit X-ray Reflectivity Analysis Software** Based on the Parrat's equation for characterization of thickness, density, and interface roughness in multialyer thin films. **Data display and export features** • Display of reflectivity profile. • Zoom and pan. • Copying of images and data profiles to Clipboard for reporting. • Layer structure display. • Exporting text data files. • Automatic HTML report creation. **Analysis features** • Simple flow bar interface. • Extended Fourier transform analysis. • Reflectivity analysis and optimization of thickness, density, and roughness using curve fitting based on a multilayer model. • Global fitting method to automatically optimize the initial fitting parameters. • Interface density or solid solution gradient modeling.	Included

ITEM	QTY	PART NUMBER	DESCRIPTION	PRICE
27	10	9289H901 9289R902	**NanoSolver SAXS Analysis Software** NANO-Solver provides size distribution functions of nano-scale pore/particles and correlation length functions for materials with density fluctuation based on the non-linear least square curve fitting analysis of x-ray small angle scattering profiles. **Features** • Slit correction to eliminate umbrella effect. Patented by Rigaku. • Pore/particle size distribution analysis using curve fitting based on a distribution function. • Pore/particle modes include spheres, plates, rods/tubes, and core/shell models. • Correlation length analysis using curve fitting based on Debye Model. For highly disordered density distributions. • Pore/particle size distribution function display in volume and number fractions. • All features list above are available for transmission and grazing incidence reflection modes. GI-SAXS modeling is patented by Rigaku. **Three different methods of analysis are available**: **Size distribution:** • The Gamma distribution function is used as the size distribution. The scattering profile is simulated based on the average size(s), volume fraction(s), and the optics configuration. **Correlation length:** • The correlation length function is used to simulate the scattering profile. The scattering profile is simulated based on the correlation length and the optics configuration. **Model free:** • The resolution function can be deconvoluted from the observed profile (the slit correction) without modeling the sample structure and the correlation function is obtained by computing the Fourier transform of the deconvoluted profile. • Mixture of multiple pore/particle size distributions or correlation functions can be modeled. • Pore/particle size distribution functions are displayed in volume and number fractions.	**Included**

ITEM	QTY	PART NUMBER	DESCRIPTION	PRICE
28	10	9220E201 9220R203	**2DP – 2 Dimensional Data Processing Software** This powerful software package integrates and processes raw 2-dimensional diffraction and scattering data collected from the detector systems. **Features** **Display:** • 2-D Image display • Pan and zoom operations • Black and white, or color display **Integration:** • Creation of intensity vs. 2θ plots • Creation of intensity vs. azimuthal angle • Automatic masking for data collected in reflection mode **Output Formats:** • PDXL, JADE, ASCII, PopLa **Pole Figure Calculation:** • From multiple images • White and Spruiell method • Stein triangle representation for polymers	**Included**
29	1	TRAIN-CUST-SITE	**Applications Training at Customer's Site** • Applications training at customer's site, 3-days by a Rigaku Applications Scientist. • Training covers basic diffraction physics, instrument operation, data reduction, and data analysis. • Training must be completed within one year of system installation.	**Included**
30	1	TRAIN TEXAS	**System Lifetime Software Training at Rigaku in The Woodlands, Texas** • PDXL software training at our regularly scheduled XRD schools. • Training available for the lifetime of the SmartLab System. • Look for schedule and request form on line at www.Rigaku.com . • Travel and lodging expenses are the customer's responsibility.	**No Charge**
31	1	TRAIN-SERVICE	**Service and Maintenance Training Class at Rigaku in The Woodlands, Texas** • At our Rigaku Service & Maintenance Training Class • 2 Days Training for up to 2 people • Travel and lodging expenses are the customer's responsibility	**Included**

ITEM	QTY	PART NUMBER	DESCRIPTION	PRICE
32	1	SERVICE	**One Year Parts Plus Service Contract** **Coverage Includes: Parts and Labor** 8:00 am to 5:00 pm, Monday through Friday, excluding Rigaku Recognized Holidays **Parts:** Parts Coverage is limited to non-consumable items. **Labor:** Labor coverage is limited to 2 service visits per year.	Included
33	1	SERVICE	**Extended Warranty – 78 months** **Includes:** • Only o X-Ray Tube o Goniometer o X-Ray Mirror	Included
			Total Section 1	**$ 531,399**
			Discount Section 1	**$-134,399**
			Total Purchase Price	**$ 397,000**

Notes:

1. **Some States, Counties, Municipalities or Provinces require Radiation Meters to be present at the time of installation. If so, this can purchased from Rigaku Americas Corporation for $2,015.**
2. **Inside delivery is not included. If inside delivery is required, an additional charge will apply.**

These Standard Terms and Conditions of Sale (the "Terms and Conditions") shall govern the sale by Rigaku Americas Corporation ("Rigaku") to the purchaser to which the Quotation is issued (the "Buyer") of the products and services (collectively, the "Goods") specified in the Quotation. The Quotation, once accepted by the Buyer as provided below, together with the Terms and Conditions form the sole agreement between Rigaku and the Buyer with respect to the purchase and sale of the Goods (the "Agreement").

Rigaku's offer to sell the Goods to Buyer, whether or not specified in Rigaku's Quotation, is expressly conditioned on Buyer's acceptance of and agreement to these Terms and Conditions. Any addition to or change in these Terms and Conditions will only be effective after Rigaku's express written agreement thereto.

1. **Price**. All prices quoted in the Quotation are valid until midnight Central Standard Time on the date set forth on the Quotation. Prices are stated in U.S. dollars unless otherwise indicated in the Quotation and are exclusive of all taxes and duties. Any sales or other tax or duty that Rigaku is required by law to collect or pay upon the sale of the Goods will be added to the invoice and paid by the Buyer to Rigaku.

2. **Payment Terms**. Unless otherwise stated in the Quotation, payment of the price for the Goods and other amounts due from the Buyer shall be due thirty (30) days from the date of invoice. A late payment charge of no more than 12% per annum (or the maximum legal rate) may be added to all invoices not paid by the specified due date. In the event that delivery of the Goods is delayed at the Buyer's request, ninety percent (90%) of the amount invoiced for the Goods shall be due on the original delivery date specified in the Quotation.

3. **Shipment and Delivery**. Unless otherwise agreed and/or specified in the Quotation, Rigaku shall ship the Goods FOB shipping point. Delivery shall be made in accordance with the terms stated in the Quotation. In the event that Buyer is unable to accept delivery of Goods on the original delivery date, including because of Buyer's failure to adequately prepare the site pursuant to Section 13 hereof, and no other arrangements have been agreed to by Rigaku and Buyer: (1) the warranty period will commence on the original delivery date; (2) if Rigaku is able to store the Goods in its own facilities, Buyer will pay Rigaku's reasonable handling, storage and insurance charges for the period of such storage; and (3) if Rigaku is unable or unwilling to store the Goods in its own facilities, it reserves the right to arrange handling and storage in a suitable bonded warehouse for Buyer at Buyer's expense.

4. **Title and Risk of Loss**. Unless otherwise specified herein and in the Quotation, title and risk of loss shall pass to Buyer at the time of shipment.

5. **Security Interest**. Buyer hereby grants, and Rigaku retains, a purchase money security interest in the Goods until all amounts due to Rigaku are paid, and Buyer agrees that it shall execute all documents necessary to secure such interest to Rigaku.

6. **Software License**. Rigaku hereby grants to Buyer a personal, non-transferable, non-sublicensable, non-exclusive limited license to use any computer software programs, specifications and related documentation in written or electronic form incorporated into or made a part of the Goods or services purchased pursuant to this Agreement, if any, for purpose of Buyer's ordinary business use of the systems included in the Goods.

7. **Warranty**. New Goods, except expendables and supplies, are warranted against defects in materials and workmanship that materially affect the functionality of the Goods until the earlier of twelve (12) months from installation or fourteen (14) months from delivery. Rigaku warrants that at delivery the Goods will conform to any written product specifications provided to Buyer. Rigaku's sole obligation under this warranty shall be, at Rigaku's option, to repair or replace defective components, including the cost of shipping parts and providing labor for installation, if applicable, or to credit Buyer's account for any Goods which are returned by Buyer during the applicable warranty period. The warranty on repaired or replaced parts and components (including labor) shall last for the remainder of the original warranty period. If the Goods (or any part or component thereof) has been disassembled, tampered with or modified by non-Rigaku personnel in any way, or has been lost, damaged, destroyed, or subjected to any abuse or misuse (whether or not intentional) following delivery or installation, or has been operated in any manner inconsistent with the applicable product specifications or instructions for use, then the foregoing warranty is void.

This warranty does not extend to other vendors' products that are supplied to Buyer in conjunction with the Goods, or are used as components or parts in the Goods. Those products are warranted by their respective manufacturer's or vendor's warranties in effect on the date of shipment to Buyer. Rigaku assigns to Buyer all rights it may have in such warranties.

THE WARRANTY SET FORTH ABOVE IS EXPRESSLY IN LIEU OF AND EXCLUDES, AND RIGAKU DISCLAIMS, ALL OTHER WARRANTIES, WHETHER EXPRESS OR IMPLIED, INCLUDING, BUT NOT LIMITED TO IMPLIED WARRANTIES OF MERCHANTABILITY, NON-INFRINGEMENT AND FITNESS FOR A PARTICULAR PURPOSE, AND CONSTITUTES THE ONLY WARRANTY OF RIGAKU WITH RESPECT TO THE GOODS.

8. **Mutual Indemnification**. Each party hereto agrees to indemnify and hold harmless the other party, including its employees, officers, directors, affiliates, partially or wholly owned subsidiaries, agents, successors and assigns, from claims for personal injury, death or damage to property (other than the Goods) arising from or in connection with the sale of the Goods due to the negligence, recklessness or willful misconduct of the indemnifying party, except to the extent of any negligence, recklessness of willful misconduct of the indemnified party. In the event that such a claim is asserted, the indemnified party will promptly notify the indemnifying party, and the indemnifying party shall have the right to assume defense of any third-party claims, provided that it conducts the defense in a reasonable manner.

9. **Insurance**. Rigaku represents that it maintains reasonable and customary insurance covering the sale of Goods.

10. **Limitation of Liability**. BUYER ACKNOWLEDGES THAT THE REMEDIES SET FORTH IN SECTIONS 7 AND 8 ARE THE SOLE AND EXCLUSIVE REMEDIES AVAILABLE TO BUYER. NEITHER RIGAKU NOR BUYER SHALL BE LIABLE FOR ANY INCIDENTAL, CONSEQUENTIAL OR SPECIAL LOSSES, DAMAGES, OR EXPENSES, DIRECTLY OR INDIRECTLY ARISING FROM THE SALE, HANDLING, INSTALLATION, SERVICE OR USE OF THE GOODS, EXCEPT WITH RESPECT TO THIRD-PARTY CLAIMS PURSUANT TO SECTION 8.

Buyer acknowledges that the Goods may include radiation and electrical sources that are inherently dangerous and could cause death, personal injury and property damage, and that the entire risk arising out of the use and performance of the Goods remains with Buyer. Accordingly, Buyer (i) acknowledges that Buyer is allowed and fully able to inspect and test the Goods before they are installed at its facility, and accordingly, assumes full responsibility for assuring they perform according to specifications and meet Buyer's requirements; and (ii) assumes full responsibility to ensure that the Goods are deployed and used by its personnel in a safe and proper manner. Under no circumstances and irrespective of the cause shall Rigaku be liable for any injury or damage to property resulting from the improper use of the Goods by Buyer or Buyer's agents.

11. **Limitation of Actions**. No action shall be brought with respect to the Goods or these Terms and Conditions more than two (2) years after the accrual of the cause of action therefor.

12. **Force Majeure**. Neither party shall be liable to the other for any delay or failure to perform which is due to any cause beyond its reasonable control. Performance times shall be considered extended for a period of time equivalent to the time lost because of any delay which is excusable hereunder. Each party will give the other party written notice within a reasonable time after becoming aware of any such delay.

13. **Site Preparation**. Buyer shall prepare the installation site at Buyer's expense, provide utilities in accordance with Rigaku's pre-installation instructions and specifications, furnish uncrating, rigging, electrical, plumbing or other assistance, as required, and furnish materials and labor for connecting specified utilities to the Goods. Failure to do so, prior to Rigaku's service personnel arriving at Buyer's site on the mutually agreed upon installation date, will result in a service charge by Rigaku to cover the lost time of its service personnel. It is the Buyer's sole responsibility to timely obtain and pay for any required authorization or registration, including X-ray registration, and to satisfy all federal, state and local safety regulations applicable to the Goods.

14. **Installation**. On-site installation and instrumentation start up are provided by Rigaku at no additional charge unless otherwise stated in the Quotation. Software applications training may be provided under a separate arrangement, unless specifically provided in the Quotation.

15. **Cancellation Policy**. If Buyer cancels or terminates this Agreement, Buyer shall be liable for payment of reasonable cancellation charges, which shall not exceed the price of the Goods cancelled, but which shall include, among other things, expenses incurred by Rigaku prior to the termination date with regard to the Goods, Rigaku's actual liabilities against commitments incident to this Agreement, properly allowable indirect charges and a reasonable profit.

16. **Amendment**. The Agreement and these Terms and Conditions may not be amended except by a separate written agreement signed by the both Buyer and Rigaku. Any provision of Buyer's request for quotation, purchase order or any other document of Buyer which is inconsistent with the foregoing shall be of no force and effect, unless Rigaku shall have expressly agreed to a modification in writing.

17. **Governing Law**. This Agreement shall be governed by and construed in accordance with the laws of the State of Texas.

18. **Assignment**. Neither party may assign this Agreement without the express written consent of the other party, which consent shall not be unreasonably withheld.

19. **Severability**. The parties agree that each provision contained in this Agreement shall be treated as a separate and independent clause, and that if one or more of these provisions shall for any reason be held excessively broad or unenforceable, such provision or provisions shall be construed by the appropriate judicial body by limiting and reducing it or them, so as to be enforceable to the extent compatible with applicable law.

20. **Waiver**. Failure by either party to exercise or enforce any rights hereunder shall not be deemed to be a waiver of any such right nor operate so as to bar the exercise or enforcement thereof at any time or times thereafter.

Entire Agreement. This Agreement represents the entire understanding of the parties with respect to the subject matter hereof and supersedes all prior agreements and understandings between them with respect to the subject matter hereof. No terms, conditions, prior course of dealings, course of performance, usage of trade, understandings, purchase orders, or agreement purporting to modify, vary, supplement or explain any provision of this Agreement shall be effective unless in writing signed by representatives of both parties authorized to amend this Agreement.

Appendix 4
Course Syllabi from Spring Semester 2016

PHYS5324: Thin Films Laboratory/MSEC7310: Nanoscale systems and devices, Spring 2016

Course Instructor: Dr. Alex Zakhidov   Office: RFM 3230   Phone: 512-245-4720
E-mail: alex.zakhidov@txstate.edu   Office Hours: T-Th 11:00-12:00 and by appointment

Cleanroom Director: Dr. Casey Smith   Office: RFM 1206   Phone: 512-245-6635
E-mail: casey.smith@txstate.edu

RSC Manager: Mr. Eric Schires   Office: RFM 3205   Phone: 512-245-1839
E-mail: es39@txstate.edu

Course Information

- **CRN 37321**
- **Class meetings:** Mon 9:30 – 10:50 RFM 3219
- **Necessary background knowledge**: Physics: Understanding of introductory physics, waves and Maxwell's equations, modern physics with quantum treatment, thermal and statistical physics. Mathematics: Advanced working knowledge through calculus and differential equations. Materials Science: basic knowledge of materials engineering, synthesis, processing and characterization. Chemistry: A basic knowledge of chemical protocols, procedures, and adherence to safety standards is necessary for this course. Computer skills: An ability to program numerical algorithms in MATLAB (or similar high-level language) and display results in graphical form.

Course Description

- **Overview:** This course is designed as hands on real-life experimental research experience with emphasis on nanoscale device fabrication. The course provides a strong background in devices with applications in nanoelectronics, photonics, micro- and nanoscale manipulation. Students are expected to form small research groups (3-4 people) to work as a team on research topics provided by Course Instructor. All research project will be carried at Nanofabrication Research Shared Space (Cleanroom) (http://www.msec.txstate.edu/Research-Programs/Nanofabrication.html) and Analysis Research Service Center (RSC) (http://www.msec.txstate.edu/Research-Programs/Analysis.html) with state-of-the-art thin film growth, processing and characterization user facilities capabilities. Following this course, students are expected to have a working knowledge of nanofabrication processing and characterization methods and demonstrated ability to apply this methods to research problems. MSEC, PhD students should expect additional load of more advanced research topics such as working photovoltaics, thin film transistors, LEDs, MBE and MOCVD.
- Tentative research topics:
  1. E-beam deposition of high quality, ultra-flat gold films on Si substrates.
  2. Carbon nanotube thin film transistors.
  3. Organohalide lead perovskite films grown on Al doped ZnO.
  4. TBA
- **Grading components**: Course grading components are research proposal, presentations (Group Reports) and final poster session.
- **Anyone who does not adhere to safety standards in the laboratory, fails to observe cleanroom rules and protocols of the facility, disregards instruction, or who engages in any kind of horseplay will automatically fail the course**.
- **Grading scale**: A=100-85%, B=84-75%, C=74-65% and D=64-50%, F=49 to 0%.

• **Textbooks:** 1. “Introduction to Physics and Technology of Thin Films” by Yuming Wang and Alfred Wagendristel, World Scientific Pub Co. 1994.
2.“Handbook of Thin Film Deposition (3rd Edition) by Seshan, Krishna, William Andrew, 2012
3. “Fundamentals of Nanoscale Thin Film Analysis” by Alford, Terry L. Feldman, Leonard C. Mayer, James W., Springer, 2007.
You do not need to purchase those text, they are available to you through the Alkek Library.
http://site.ebrary.com/lib/txstate/reader.action?docID=10700664
http://site.ebrary.com/lib/txstate/reader.action?docID=10578531
http://site.ebrary.com/lib/txstate/reader.action?docID=10229136
You *do not* have permission to print using university printers.

Tentative Course Schedule with Tentative Content

Month	Week	Workshop	Laboratory
January			
	KW3	Introduction to thin film science	Online Safety Training
	KW4	Competitive research proposal writing	Introduction to Safety and Cleanroom Practices + Facility Walkthrough
February	KW1	Vacuum Technology	Vacuum Controllers, Hardware, and System Operation Furnace
	KW2	Thin Film Metrology	Thermal and e-beam vacuum deposition
	KW3	**Proposal submission and review**	(Thermal) Oxidation of Silicon
	KW4	**Group report.** Physical Vapor Deposition	RF Sputtering
March	KW1	**Group report**. RF Sputtering	Scanning Electron Microscopy
	KW2	**Group report**. Thermal Processing	Scanning Electron Microscopy/EDX
	KW3	**Group report**. SEM	Atomic Force Microscopy
	KW4	**Group report**. AFM	Atomic Force Microscopy
April	KW1	**Group report**. X-Ray analysis	XRD/XRR
	KW2	**Group report**. TBA	XRD/XRR
	KW3	**Group report**. TBA	Impedance spectroscopy
	KW4	**Group report**. TBA	TBA
			TBA
May	05/11	Final Exam/Poster Session (3:00-5:30 PM)	

TEXAS STATE UNIVERSITY POLICIES:

You are expected to know Texas State's rules concerning Academic Honesty. You can get information on Academic Honesty from the Dean of Students Office or your instructor or your copy of the Texan State student handbook. Academic dishonesty will not be tolerated and will be treated according to the university honor code.

Texas State Academic Honor Code

As members of a community dedicated to learning, inquiry and creation, the students, faculty and administration of our university live by the principles in this Honor Code. These principles require all members of this community to be conscientious, respectful and honest.

WE ARE CONSCIENTIOUS. We complete our work on time and make every effort to do it right. We come to class and meetings prepared and are willing to demonstrate it. We hold ourselves to doing what is required, embrace rigor, and shun mediocrity, special requests, and excuses.

WE ARE RESPECTFUL. We act civilly toward one another and we cooperate with each other. We will strive to create an environment in which people respect and listen to one another, speaking when appropriate, and permitting other people to participate and express their views.

WE ARE HONEST. We do our own work and are honest with one another in all matters. We understand how various acts of dishonesty, like plagiarizing, falsifying data, and giving or receiving assistance to which one is not entitled, conflict as much with academic achievement as with the values of honesty and integrity.

E-mail Communication

All e-mail communications for this course, no matter who are the participants in the exchange, should be professional. Do not use text message abbreviations and other shortcuts. Write in complete sentences and use only jargon specific to the course.

Put your course number (PHYS5324/MSEC7310) in the subject line along with a description of the content. Putting the course number in the subject allows your instructor to respond to you in a timely manner.

A Texas State email address is a course requirement. If you send to the instructor you must use your Texas State email address, for example, zzz99@txstate.edu. This is University policy. Messages from other email services will not be read. If you are not at a University computer, emails can be sent via Texas State Bobcat Mail (go to www.txstate.edu and select bobcatmail).

University policy discourages sending grade information via email. Use office hours to discuss grading and to go over exams.

Special Needs

Students with special needs (as documented by the Office of Disability Services) should identify themselves at the beginning of the semester. Students with special testing accommodations will take their tests at Disability Services in the LBJ Center. Please see the instructor at least a few days before the test to make sure everything is in order and that a test will be available for you. Disability Services requires that signed forms be presented to them at least two business days before the test is scheduled.

Dr. Nikoleta Theodoropoulou RFM 3215 ntheo@txstate.edu

MSEC 7311 Materials characterization – Spring 2016

Class Times & Location:	T Th, 12:30 – 1:50, RFM 4236
Catalog Description:	This course covers skills and knowledge required for microscopy methods including transmission electron microscopy, scanning electron microscopy, scanning tunneling electron microscopy, atomic force microscopy, and confocal microscopy. It covers x-ray and neutron diffraction techniques including structure analysis, powder and glancing angle diffraction, pole figure, texture analysis, and small angle scattering.
Textbook:	*Materials Characterization - Introduction to Microscopic and Spectroscopic Methods (2nd edition) by Leng, Yang,* ISBN:9783527334636. **It is available to you online through the TX STATE library at no-cost: http://site.ebrary.com/lib/txstate/detail.action?docID=10301127**
Instructor:	Dr. Nikoleta Theodoropoulou, e-mail: ntheo@txstate.edu, Office phone: 245-5584
Course Outline	1. Optical Microscopy 2. Ellipsometry 3. Scanning Probe Microscopy – Atomic Force Microscopy, Scanning Tunneling Microscopy, Magnetic Force microscopy… 4. X-ray diffraction 5. Scanning Electron Microscopy 6. Single crystal structure analysis 7. X-Ray Spectroscopy 8. Electron Spectroscopy 9. Other techniques: Neutron Diffraction, …
Grades:	Grades will be determined by a combination of traditional exams and quizzes, and assigned lab exercises and homework. Exams and Quizzes 40% Lab Assigned Research 40% Final Research Lab and Lab report 20% The final exam is comprehensive and will be given as an out of class assignment during finals week.
Attendance:	You are expected to attend class with proper preparation. If you know in advance of unavoidable absences, please communicate these with the instructor well in advance to mitigate the effect of them. Office hours: T Th 2:00 – 3:00 (subject to change) or by appointment (email preferable) **Class information is available on TRACS**
Special Needs:	Students with special needs, as documented by the Office of Disability Services, should identify themselves at the beginning of the semester. Arrangements can be made to accommodate those needs as necessary.
Grading Scale:	The minimum grading scale is given below but may be adjusted at the end of the course to account for a low average. 90% - 100% A 80% - 89% B 70% - 79% C 60% - 69% D below 60% F